Model Description for ACC-HUMANsteady 1.0

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# General Structure of the ACC-HUMANsteady Bioaccumulation Model

The bioaccumulation model is designed as a steady-state model relying on mechanistic process descriptions. The model is subdivided into an aquatic food web (plankton, benthos, planktivorous fish, piscivirous fish), an agricultural food chain (grass, milk cow, beef cattle), four different types of crops/cultivated plants (leafy vegetables, root fruits, aerial fruits, and tubers), and the human as the top consumer and model endpoint. In addition to the dietary uptake, the model considers direct exposure to contaminants present in the physical environment via respiration, drinking and ingestion of soil or sediment particles. Elimination pathways considered for each organism are excretion via feces, respiration, metabolism, growth, and for mammals additionally urination, percutaneous excretion, and in the case of females, loss via birth and lactation. For the vegetation, contaminant uptake from both soil and the atmosphere is considered, as well as contaminant loss due to biotransformation, due to growth, and loss to the atmosphere. The model structure is illustrated in Figure .

The steady state approach has been widely applied in bioaccumulation models for the aquatic environment, e.g.[1,2]. The models generally predict the chemical levels in the organism of different trophic positions within a satisfactory range of agreement with field data, at least if the focus is set on an estimation of the average exposure of top-predators relying on a diet consisting in a varying composition of different fish species and aquatic invertebrates, e.g. [1,3]. Also for the terrestrial environment and lung-breathing organisms, the steady-state approach is applied in many of the existing bioaccumulation models, e.g. [4-7]. However, in some cases steady state models are not suitable. For instance, in long-living top-predators such as humans and seals the time required for persistent lipophilic chemicals to approach steady-state can be far in excess of the organisms’ lifetime. In judging whether a steady state model can be applied to a given situation, the key consideration is whether the assumptions of constant chemical concentrations in exposure media and constant environmental properties are valid over the time period that it would take the organism to approach steady state. To aid the user in making this judgment, the model calculates the time it would take for each organism to approach 90% of steady state (see equation below). The user can compare this number with the expected time scale for trends in the relevant chemical concentrations in exposure media and environmental parameters to make a qualitative evaluation of the applicability of the steady state model.

|  |
| --- |
| model structure 2bc |

**Figure** **1.** A) Structure of the bioaccumulation food web model. The arrows symbolize the contaminant uptake from the physical environment and the contaminant transfer within the food web; B) general uptake and elimination processes considered for the fauna; C) general uptake and elimination processes considered for plants.

Fugacity approach. The process descriptions are based on the fugacity approach [8]. The chemical concentration C (mol m-3) in a given phase is expressed as the product of the fugacity capacity Z (mol m-3 Pa-1), which is a measure for the capacity of the phase to store or retain the given chemical, and the fugacity f (Pa), which can be viewed as the partial pressure of the chemical in the phase. Equilibrium partitioning between two phases *i* and *j* is achieved when the fugacities are equal in both phases. Consequently, the partition coefficient Kij is the ratio of the Z values of phases *i* and *j*. The temperature dependence of Kij and of the corresponding Z values can be described with the van’t Hoff equation:

 (1)

where T and T0 are the ambient and the reference temperatures (K), respectively, Uij is the internal energy (kJ mol-1), and R is the gas constant (8.314 J mol-1 K-1)).

Both diffusive and advective chemical transport processes are expressed with so called D values (mol d-1 Pa-1), which are the product of a flow rate G (m3 d-1) and a fugacity capacity. For each (interconnected) compartment *i*, a mass balance of the form

 (2)

is written, in which V is the volume (m3), and the index *j* stands for an interconnected adjacent compartment; the first index of the D value identifies the compartment the chemical is coming from, and the second its destination. At steady state, eq. can be simplified to:

 (3)

Integrating and re-arranging eq. gives the time t90 (d) needed for an uncontaminated body (fi0 = 0) to reach 90% of a steady-state contaminant level:

 (4)

If the calculated t90 is higher than the assumed life time of the organism, the model makes the following correction of the fugacity (i.e. the analytical solution of the differential equation is used):  (5)

where t is the life time of the organism.

# Physical Environment

The model can be easily linked to multimedia fate and transport models, allowing a sophisticated estimation of the contaminants distribution in the environment and the exposure of wildlife and humans as the result of chemical emissions. Alternatively, the user can directly define environmental concentrations or fugacities which are used as input for the bioaccumulation model. For this purpose, a tool is provided to calculate environmental fugacities from given concentrations or, alternatively, from a level I unit world, consisting of an air compartment including aerosols, a water compartment including suspended matter, a sediment compartment, and a soil compartment. The default parameterization is set in accordance with the regional default scenario of EUSES (Table 1)[9]; the size and the suspended solid content of the water and soil compartments are calculated as weighted mean values of the three soil and two water compartments in the regional default scenario of EUSES[9].

Each compartment (bulk air, water, soil, sediment) and sub-compartment (aerosols, suspended matter) in the physical environment is described as a homogeneous mixture of different phases (e.g. water and organic carbon), in which chemical equilibrium partitioning is assumed within each compartment. The equations for the calculation of the fugacity capacities of the abiotic phases and compartments and the corresponding partition coefficients of aerosols, suspended matter, sediment and soil are given in Table 2. In accordance with [9] and the Technical Guidance Document (TGD)[10], the default algorithm for the organic carbon-water partition coefficient KOC is the sp-LFER suggested in [11] for non-polar organic chemicals. In addition to the general sp-LFER, chemical group specific sp-LFERs are provided in this work, which have a higher prediction accuracy compared to the general equation. The user is encouraged to use the equation for the chemical group investigated. For the aerosol-air partition coefficient KQ, the approach suggested by [12] was adopted.

**Table 1.** Default parameterization of the physical environment in accordance with [9].

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | **total environ.** | | | **air** | | **aerosols** | **water** | **susp. matter** | **soil** | **sediment** |
| area [km2] | 4.04∙104 | | | 4.04∙104 | |  | 1.62∙103 |  | 3.88∙104 | 1.62∙103 |
| depth [m] |  | | | 1000 | |  | 4.73 |  | 0.14 | 0.03 |
| volume [km3] |  | | | 4.04∙104 | |  | 7.64 |  | 5.43 | 0.05 |
| volume fractions *v* [m3 m-3]: | | | | | | | | | | |
| particles in bulk phase | | |  |  | | 2∙10-11 |  | 8.42∙10-6 |  |  |
| Solids | | |  |  | |  |  | 0.1 | 0.6 | 0.2 |
| Water | | |  |  | |  |  | 0.9 | 0.2 | 0.8 |
| Air | | |  |  | |  |  |  | 0.2 |  |
| mass fraction [g g-1] | | | | | | | | | | |
| OC in solids | | |  |  | | 0.04 |  | 0.1 | 0.02 | 0.05 |
| Densities ρ[kg m-3] | |  | | |  | | | | | | |
| aerosols (Q) | | 2260 | | | [12] | | | | | | |
| octanol (O) | | 820 | | | [12] | | | | | | |
| solid phase | | 2500 | | |  | | | | | | |
| organic matter (OM) | | 1000 | | |  | | | | | | |
| bulk susp. Matter (SS) | | 1150 | | |  | | | | | | |
| bulk soil (E) | | 1700 | | |  | | | | | | |

**Table 2.** Fugacity capacity Z of the abiotic phases in (mol m-3 Pa-1); R is the gas constant (8.314 J mol-1 K-1), H is the Henry Law’s constant (m3 Pa mol-1), and T is the ambient temperature (K).

|  |  |  |  |
| --- | --- | --- | --- |
|  | **Z-value** | **sp-LFER** | **Ref.** |
| air (A) |  |  |  |
| water (W) |  |  |  |
| octanol (O) |  |  |  |
| aerosols (Q) |  | [m3 m-3] Note: in the original work, ρQ was used instead of ρOC | [12] |
| bulk susp. matter (SS) |  | [L kgOC-1] | [11] |
| susp. matter solids |  |  |  |
| bulk sediment (S) |  | [L kgOC-1] | [11] |
| sediment solids |  |  |  |
| bulk soil (E) |  | [L kgOC-1] | [11] |
| soil solids |  |  |  |

# Biota

The bioaccumulation model is based on ACC-HUMAN, a fugacity based food chain model predicting human exposure to organic contaminants from environmental levels [13]. It also includes models of uptake in plants developed by Trapp [6], and models of uptake in benthic organisms developed by Morrison and co-workers [14]. The model relies on mechanistic process descriptions, assembling mechanistic knowledge from published research on bioaccumulation in different food chains and trophic levels.

All biota (identifier b) apart from plants and plankton are described with two-compartment models distinguishing between the gastrointestinal tract and the organism itself. Chemical equilibrium partitioning between all tissues is assumed. The fugacity capacity of the organism is calculated as the volume weighted sum of the capacities of the different tissues *i*:

 (6)

The fugacity capacity of lipids is assumed to be equal to that of 1-octanol; the Z value of non-lipid organic matter (NLOM) such as proteins and carbohydrates is expressed as a fraction β of the octanol Z-value. In a first approximation, β is set to 0.035 as suggested by Arnot and Gobas [15]. The tissue content of lipids (lip), water (W), non-lipid organic matter (NLOM), and, in the case of plants, also air (A) is considered (see Table 3), yielding the general equation for the biota Z-value:

 (7)

The lipid normalized concentrations (g glip-1) of the biota are calculated according to equation 8:

 (8)

**Table 3.** Composition of the tissues considered to contribute to the overall storage reservoir for organic chemicals in the biota.

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | **units** | **lipid** | | **NLOM** | | **water** | **air** | **Ref.** |
|  |  |  | | **protein** | **carbo- hydrates** |  |  |  |
| **Woman (30yr)** | [g g-1] | 0.38\* | | 0.06\* | | 0.44\* |  | [16] |
| **Human milk** | [g g-1] | 0.044 | | 0.079 | | 0.87 |  | [17] |
| **Infant** | [g g-1] | 0.29\* | | 0.07\* | | 0.52\* |  | [16] |
|  |  | \* Function of age | | | | |  |  |
| **Vegetation** |  |  | |  | |  |  |  |
| **leaf** | [m3 m-3] | 0.01 (includes all organic sorbing phases) | | | | 0.7 | 0.29 | [13,18,19] |
| **root** | [g g-1] | 0.025 | | 0.01 | 0.08 | 0.885 | 1.3∙10-4 | [6,7,20] |
| **root fruit** | [g g-1] | 0.025 | | 0.01 | 0.08 | 0.885 | 1.3∙10-4 |  |
| **apple  (aerial fruit)** | [g g-1] | 0.006 | |  |  | 0.844 | 3.25∙10-4 | [6] |
| **grain (aerial fruit)** | [g g-1] | 0.03 | | 0.10 | 0.70 | 0.17 |  |  |
| **tuber** | [g g-1] | 0.001 | | 0.02 | 0.199 | 0.78 |  | [21] |
| **transpiration flow** | [m3 m-3 ] |  | |  | | 1 |  |  |
| **phloem flow** | [m3 m-3 ] |  | |  | 0.1 | 0.9 |  | [22] |
| **Grass** | [m3 m-3 ] | 0.01 (includes all organic sorbing phases) | | | | 0.7 | 0.29 |  |
| **Cattle(beef/milk)** | [g gcattle-1] | 0.2 | | 0.16 | | 0.56 |  | [23] |
|  | [g gsorbing matrix-1] | | 0.22 | 0.17 | | 0.61 |  |  |
| **milk** | [g g-1] | 0.05 | | 0.08 | | 0.87 |  | [24] |
| **Dairy products** | [g g-1] | 0.33 | | 0.29 | | 0.38 |  |  |

**Table 3 (continued).**

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  |  |  | | | | | |  |
|  | **units** | **lipid** | | **NLOM** | | **water** | **air** | **Ref.** |
|  |  |  | | **protein** | **carbo- hydrates** |  |  |  | |
| **Zooplankton** | [m3 m-3] | | 0.05 | 0.2 | | 0.75 |  | [13,15] |
| **Benthos** |  |  | |  | |  |  |  |
| **b1** | [m3 m-3] | 0.05 | | 0.2 | | 0.75 |  | [13,15] |
| **b2** (filter feeder) | [m3 m-3] | 0.03 | | 0.17 | | 0.8 |  | [25] |
| **b3** (deposit feeder / predator) | [m3 m-3] | 0.02 | | 0.2 | | 0.78 |  | [15,26,27] |
| **Fish 1** (planktivore) | [m3 m-3] | 0.035 | | 0.265 | | 0.7 | 0 | [13,28,29] |
| **filet** | [m3 m-3] | 0.035 | | 0.265 | | 0.7 | 0 | [13,30] |
| **Fish 2** (piscivore) | [m3 m-3] | 0.044 | | 0.256 | | 0.7 | 0 | [13,28,29] |
| **Filet** | [m3 m-3] | 0.005 | | 0.295 | | 0.7 | 0 | [13,30] |
| **Densities:** |  |  | |  | |  |  |  |
|  | [kg L-1] | 0.92 | | 1.0 | | 1.0 | 1.3∙10-3 | [16,31] |

## Bioconcentration, bioaccumulation and biomagnification factors.

The bioconcentration factor BCF is a measure of the bioaccumulation resulting from exposure via respiratory surfaces, e.g. via gill ventilation. The BCF is equal to the (density corrected and lipid normalized) concentration ratio between the organism Zbiota∙fbiota and the ambient medium Zenv∙fenv under laboratory conditions:

 (9)

where ρlip is the lipid density and vlip\_b is the lipid volume fraction of the organism (Table 3).

The bioaccumulation factor BAF is a measure for the exposure from both respiratory and dietary pathways, defined as the (observed) concentration between organism and ambient medium:

 (10)

The biomagnification factor BMF is a measure of the fugacity increase along a food chain and can be expressed as the fugacity ratio between predator and prey. Often the BMF is reported as the fugacity ratio to individual prey items. This does, however, not reflect the contribution of the given prey item to the overall exposure of the organism. In this model, an overall BMF is calculated which is calculated on the basis of the weighted mean prey fugacity according to the dietary preferences (Table 11):

 (11)

 (12)

The multimedia bioaccumulation factor mmBAF is a measure of the exposure of an organism to the total quantity of chemical in the multimedia environment (normalized to 1 m2) the organism is living in [32]:

 (13)

In contrast to the BAF, the mmBAF accounts for simultaneous exposure from different abiotic phases. Humans, for example, is directly exposed to chemicals in air and water via inhalation and drinking, but also indirectly by consumption of food originating from both aquatic and terrestrial biota. With units of m2 organism-1, the mmBAF can be viewed as the surface area of the environment containing the same amount of chemical as having been accumulated in the organism. In this model, the mmBAF is calculated if the optional Level I environmental fate model is used.

**Table 4.** D values in (mol d-1 Pa-1) for contaminant uptake and elimination. Details about the definition of the parameters are given in the text and in Tables 5-11.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Process** | | **Organism** | | | **Equation** | |
| Ingestion | | all biota | | |  | |
| Egestion | | human | | |  | |
| Egestion | | fish | | |  | |
| Transfer across  intestinal wall | | cattle | | |  | |
| Urination | | mammals | | |  | |
| Respiration | | mammals | | |  | |
| Gill ventilation | | fish, benthos | | |  | |
| Percutaneous excretion | | human | | |  | |
| Lactation | | cattle | | |  | |
| Child birth | | woman | | |  | |
| Metabolism (fauna) Biotransformation (flora) | | All biota | | |  | |
| Growth | | all biota | | |  | |
| Gaseous deposition | all plant leaves and aerial fruit cuticle | |  | | | |
| Particle bound deposition | | all plant leaves | | | |  |
| **Table 4 (continued).** | |  | | |  | |
| **Process** | | **Organism** | | | **Equation** | |
|  | |  | |  | | |
| Transport with transpiration stream into leaves | | all plants | |  | | |
| Transport with transpiration stream into fruits | | aerial fruits | |  | | |
| Transport with phloem  into roots | | all plants | |  | | |
| Transport with phloem  into fruits | | aerial fruits | |  | | |
| Soil water – tuber exchange | | tuber | |  | | |

## Human

Endpoint of the model simulations is the chemical concentration in humans as a consequence of (secondary) dietary exposure from different food sources (see below the treatment of the underlying aquatic and agricultural food chains including crops), as well as via direct uptake from the physical environment via inhalation and drinking. Input for the human module are the chemical concentrations in the food items predicted with the bioaccumulation model. The endpoint is set to a 30 year old woman.

The human module is designed as a two-compartment model (gastrointestinal tract and the body itself) adopting the approach presented in [13]. Considering contaminant uptake with the diet, drinking water and inhaled air, as well as contaminant elimination due to egestion (E), exhalation (re), metabolism (M), percutaneous excretion (P), urination (ur), nursing (L), childbirth (child), and growth (G), the human fugaciy fH is calculated as

 (14)

where H stands for the human, E0 is the efficiency of chemical absorption in the gastrointestinal tract, Ui is the ingested food item i, fA is the fugacity of the ambient air, and V (m3) is the volume of the human body considered to contribute to the overall sorbing matrix. The D values are defined in Table 4. Respiration is defined as a diffusive process, i.e. the D values for inhalation and exhalation are identical (Dre). A detailed description of the human model is given in [13]; the parameterization of the model is presented in Table 5. In the following, only the major features are briefly described, as well as modifications to the original model.

*Body mass & composition.* The body mass as a function of age is estimated using the equation given in [33] for girls/women. Following the approach given in [13,34], the lipid mass is calculated using the estimates for the lipid content as a function of age given in [35]. In addition to the lipids, non-lipid organic matter (NLOM) and water are assumed to build up the sorbing matrix of the human body. The water content is set to 71% of the lipid free body mass [13], and 9% of the lipid free body mass is assigned to the non-lipid organic matter (the remaining 20% of the lipid free body mass are composed of the skeleton which is not accounted for as part of the sorbing matrix) (Table 3). The Z value for the human body is calculated applying equation 7.

*Ingestion & chemical absorption.* The food groups considered as potential sources of secondary exposure to organic chemicals are dairy products, beef, fish, and vegetables. The latter are subdivided into four sub-groups in dependence of the kind of the edible part of the plant: two aerial groups (leafy vegetables such as lettuce, and aerial fruits such as apples, but also cereals), and two subterraneous groups (root vegetables such as carrots, and tubers such as potatoes). The ingestion rates are defined as a function of age on the basis of studies on the food consumption studies of Swedish children in 2003 [36] and of Swedish adults in 1997-98 [37], (Table 5). The dairy products were summarized as the weighted mean value on the basis of the lipid contents. The total daily grain

**Table 5.** Parameterization of the human module in accordance with [13].

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | **Unit** | **symbol** | **value / equation** | **Ref.** |
| Age | [yr] | tH | 30 |  |
| Ingestion rates: |  |  |  |  |
| Water | [m3 d-1] | GUW\_H |  | [36,37] |
| Fish | [g ww d-1] | GUF\_Hww |  | [36,37] |
| Dairy products | [g ww d-1] | GUMC\_Hww |  | [36,37] |
| Beef | [g ww d-1] | GUBC\_Hww |  | [36,37] |
| Vegetable 1 (aerial fruit) | [g ww d-1] | GUV1a\_Hww |  | [36,37] |
| Vegetable 1 (grain) | [g ww d-1] | GUV1b\_Hww |  | [36,37] |
| Vegetable 2 (tuber) | [g ww d-1] | GUV2\_Hww |  | [36,37] |
| Vegetable 3 (leafy) | [g ww d-1] | GUV3\_Hww |  | [36,37] |
| Vegetable 4 (root) | [g ww d-1] | GUV4\_Hww |  | [36,37] |
| Absorption efficiency |  | E0\_H |  | [13,34] |
| Feces dry weight excretion | [g dw d-1] | G’F\_Hdw |  | [34] |
| Feces-blood partition coefficient | [m3 body lipid / g feces dw] | KFB | non-planar molecules: 2∙10-8  planar molecules: 8∙10-8 | [65] |
| **Table 5 (continued).** |  |  |  |  |
|  | **Unit** | **symbol** | **value / equation** | **Ref.** |
|  |  |  |  |  |
| Water excretion rate | [m3 d-1] | Gur\_H |  |  |
| Percutaneous body lipid excretion rate (30yr old) | [m3 d-1] | GP\_H | 7.78∙10-7 | [13] |
| Inhalation rate (30yr old) | [m3 d-1] | Gre\_H | 15 | [13] |
| Metabolism rate constant | [d-1] | kM\_H | Chemical dependent |  |
| Growth rate constant | [kg yr-1] | kG\_H | 0.2 |  |
|  |  |  |  |  |
|  |  |  |  |  |

consumption rate was estimated as the weighted mean value of bread, porridge and cereal on the basis of the estimated grain contents (0.72, 0.5, and 0.75, respectively). The consumption of fruits includes the consumption of juice. The composition of the sorbing matrix of the different food groups is listed in Table 3.

The chemical fugacity of the food categories fUi is calculated from the predicted fugacity in the original food item fUi0 (e.g. fugacity in dairy products from fugacity in the cow milk) by taking the different fugacity capacities and thus volume fractions of lipids, NLOM, and water into consideration and assuming a density of 1000 kg m-3 for each:

 (15)

The chemical absorption in the digestive tract is based on the model presented in [34], considering the bi-directorial chemical exchange over the gut membrane. The chemical absorption efficiency E0H is described as a function of the feces-human body partition coefficient KFB with units of [m3 body lipids / g feces dw] and the KOW by applying the two-resistance concept with a water phase and lipid phase resistance at the intestinal tract membrane. In the original work, only hydrophobic chemicals were considered, and the storage compartment of the human body was consequently assumed to consist of lipids only. Since polar chemicals are part of the domain of this model, non-lipid tissue can also be important, and hence the original KFB definition was corrected by the Z-value ratio between body lipids and the human body. The equation for E0H is given in Table 5.

*Egestion.* Based on the work of Moser and McLachlan [34], the dry weight egestion rate G’F\_Hdw is set to 10% of the dry weight ingestion rate G’U\_Hdw (Table 5). The chemical desorption efficiency is assumed to be equal to the absorption efficiency E0H (Table 4).

*Inhalation.* Chemical uptake and elimination via in- and exhalation are described as a diffusive exchange process, in which 70% of the inhaled air is assumed to reach the aveoli and equilibrate with the blood (i.e. with the human body) [13,38]. The inhalation rate Gre\_H is assumed to follow the same trend as the dry weight total diet ingestion rate, which is defined by adopting the methods described in [34] and in [13].

*Percutaneous excretion.* The percutaneous lipid excretion rate GP\_H for an adult is set to   
7.78∙10-7 m3 d-1 based on [13,39].

*Metabolism.* Metabolism is described as a first order reaction. The rate constants kM\_H (d-1) are chemical dependent and user defined.

## Agricultural Food Chain

### Grass.

Constituting the main vector of cattle exposure to organic chemicals, grass is the major link for the uptake of these contaminants from the physical environment into the agricultural food chain [40]. The grass module is designed on the basis of the non-steady state grass model presented in [13]. It is, however, designed as a steady-state model and sub-divided into two compartments, distinguishing between the root system and the aerial part as suggested in e.g. [20]. The chemical uptake and elimination processes considered in the model are diffusive gaseous exchange between the leaf compartment and the atmosphere, particle bound wet and dry deposition, uptake from the soil water with the transpiration stream, biotransformation in both the leaf and the root compartment, and chemical dilution due to growth of both compartments. The root and the leaf compartments are interconnected by the transpiration stream and the phloem flow (see below). Applying equation , the fugacities in the grass leaves fLF\_Gr and in the root system fR\_Gr are thus given by

 (16)

 (17)

where Gr, LF, R, A, and S stand for grass, leaf, root, air, and soil respectively, and the indices tr, ph, Ga, Pa, G, and M stand for the transpiration stream, the phloem flow, gaseous deposition, particle bound wet and dry deposition, growth, and biotransformation. The equations for the D-values are given in Table 4 and further explained below. The parameterization of the grass model is based on the parameterization given in [13] for rye grass (*Lolium multiflorum*) as representative for pasture grass (Table 6). Rye grass is one of the most important pasture grass species in the temperate Europe and particularly well investigated. The model is written to describe the uptake in a 1 m2 plot of pasture. The root and leaf weight are set to 2 kg m-2, corresponding to a volume of 2.2∙10-3 and 2.6∙10-3 m3 m-2, respectively [19]. The density of grass leaves is set to 750 kg ww m-3 [13]; the density of roots is set to 900 kg ww m-3 [20].

The leaf and root tissues are described as a homogeneous mixture of organic material, air, and water, in which the organic material in the root tissue is further subdivided into lipids, proteins, and carbohydrates in accordance with [20] (Table 3). The Z-value of root lipids are derived from the lipid-water partition coefficient Klip (m3 m-3) which is modelled as a function of log KOW [41]:

Klip = 1.22 KOW0.77 (18)

The Z-values of proteins and carbohydrates are derived from the protein-water partition coefficient Kprot (m3 m-3) and the carbohydrate-water partition coefficient KCHO (m3 m-3), both of which have been defined as a function of KOW [42] (Table 6). This yields for the Z values of the leaf compartment ZLF\_Gr and the root system ZR\_Gr:

 (19)

 (20)

where v stands for volume fraction, the indices A, W, lip, prot, and CHO stand for air, water, lipid, protein, and carbohydrates, respectively and KPA is the dimensionless leaf organic matter-air partition coefficient. In the original studies from Kömp and McLachlan, KPA was defined as the plant(leaf)-air partition coefficient [43,44]. However, the authors measured the partitioning between air and the aerial part of grass and herbs exclusively for hydrophic and rather involatile organic chemical, i.e. for chemicals which sequester almost entirely into the organic matrices. Consequently, an extrapolation of the resulting plant Z value towards more hydrophilic and/or more volatile compounds requires additional consideration of the contribution of the air and water fractions in the leaf to the overall sorption capacity. Kömp and McLachlan showed that KPA can be expressed as a function of KOA, but that the heat of phase transfer between the plant tissue and air differed highly from that between 1-octanol and air [44]. To minimise the error in extrapolating KPA to different temperatures, Czub and McLachlan recalculated the correlation between KPA and KOA for the data measured at the temperature closest to the mean temperature during the growing season (9.8°C) [13,44]. This correlation was adopted for the grass model (Table 6).

*Transpiration stream.* The flow rate of the transpiration stream is set equal to the plants average transpiration rate. Due to its negligible content of organic material, it is modelled as a pure water phase. Following the approach given in [13], the transpiration stream is assumed to have the same fugacity as the soil water when entering the root system via the fine roots which are characterized by a small diameter but high surface area (i.e. roots and soil water / bulk soil are assumed to be in equilibrium). In the thick roots, the transpiration stream is then assumed to equilibrate with the root tissue before leaving the root compartment for the leaf compartment.

*Root uptake.* Chemical uptake with the roots and transport with the xylem sap into the leaves is an important pathway of the plant exposure, in particular for the rather hydrophilic substances. In principal, two uptake mechanisms can be distinguished: diffusion over the root surface, and advective transport with the transpiration stream. The more hydrophobic organic substances have a high tendency to sorb to the organic phase in the roots and are thus no subject to further translocation after having entered the roots [7], whereas the hydrophilic chemicals are efficiently transported with the transpiration stream. This makes the contribution of the diffusive uptake to the overall plant exposure negligible.

A common way to describe the efficiency of chemical transport from the external soil water to the transpiration stream leaving the roots and entering the leaves is the concentration ratio between the soil water and the transpiration stream, also called the transpiration stream concentration factor TSCF. Briggs and co-workers [45] derived a bell shaped correlation between the TSCF and the KOW, which has been widely used in plant bioaccumulation models, e.g. [5,9,13], but which has also been controversial discussed due to the predicted declining efficiency towards low KOW values. Trapp [6] showed with a steady-state root model, that the consideration of growth dilution in addition to the chemical elimination with the transpiration stream yields a similar trend of a decrease in the transfer efficiency with increasing KOW as the correlation given in [45], but a constant level for low KOW compounds. A similar approach is applied in this model, considering growth and metabolism as elimination pathways. Rearranging equation 17 gives the translocation efficiency as the fugacity ratio between the transpiration stream leaving the roots and the soil:

 (21)

DG\_RGr and DM\_RGr are dependent on the fugacity capacity of the entire root (Table 4), i.e. the D values are increasing with the KOW, which implies a decrease of the transfer efficiency. For low KOW values on the other hand it is only the relatively small water fraction in the roots and the transpiration stream itself, modelled as water only, which determine the fugacity ratio, i.e. the translocation efficiency is at a constant level close to one.

*Atmospheric deposition.* Gaseous and particle bound deposition are treated as separate vectors of exposure, the former as a diffusive exchange occurring in parallel through the stomata and the cuticle, the latter as an advective process.

Gaseous exchange through the cuticle considers the subsequent transfer from the atmosphere to the leaf surface and further into the storage compartment of the leaf, each of which is described with a mass transfer coefficient with units of m d-1 (k’gg\_Gr, and k’gp\_Gr, respectively). k’gg\_Gr is parameterized based on measurements of deposition to the plane of the canopy (ACP\_Gr) of pasture land in Germany, [46]; k’gp\_Gr is defined based on laboratory data on contaminant transport in rye grass, i.e. the k’gp\_Gr

**Table 6.** Parameterization of the grass module in accordance with [13].

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
|  | **Unit** | | **symbol** | | **value / equation** | **Ref.** | |
| leaf organic matter-air partition coefficient | [m3 m-3] | | KPA | |  | [13,44] | |
| protein-water and carbohydrate-water partition coefficients (roots) | [m3 m-3] | | KProt and KCHO | | 0.1 for Log KOW < 0, 0.2 for log KOW = 0.1 to 0.9, 0.5 for log KOW = 1 to 1.9, 1 for log KOW = 2 to 2.9, 2 for log KOW = 3 to 3.9, 3 for log KOW ≥ 4 | [42] | |
| protein-water partition coefficients (fruits) | [m3 m-3] | | KProt | |  | [20,47] | |
| carbohydrate-water partition coefficients (fruits) | [L kg-1] | | KCHO | |  | [20] | |
| Gaseous deposition: |  | |  | |  |  | |
| Deposition velocity (air-side) | [m m-2CP d-1] | | k’gg\_Gr | | 192 | [46] | |
| Deposition velocity (plant-side) | [m m-2LF d-1] | | k’gp\_Gr | | 6.72∙10-7 | [19,48] | |
| Stomatal mass transfer coefficient | [m d-1] | k’stom\_Gr | | where MW is the chemical’s molecular mass (mol g-1), rh is the rel. humidity (set to 0.5), and T is the ambient temperature in (K) | | | [6] |
| Particle bound deposition: |  | |  | |  |  | |
| Deposition velocity (wet & dry) | [m m-2CP d-1] | | k’p\_Gr | | 72 | [46] | |
| Flow rates: |  | |  | |  |  | |
| Transpiration rate | [m3 m-2LF d-1] | | Gtr\_Gr | | 2.4∙10-4 | [13] | |
| Area: |  | | | | |  | |
| Canopy | [m2] | | ACP\_Gr | | 1 |  | |
| Leaves | [m2 m-3LF] | | ALF\_Gr | | 5000 | [13] | |
| Volume: |  | |  | |  |  | |
| Roots | [m3 m-2CP] | | VR\_Gr | | 2.2∙10-3 |  | |
| Leaves | [m3 m-2CP] | | VLF\_Gr | | 2.6∙10-3 | [19] | |
| Root density | [g m-3] | | ρroot\_vx | | 9∙105 | [20] | |
| Growth rate constants: |  | |  | |  |  | |
| Roots | [d-1] | | kG\_RGr | | 0.035 | [6] | |
| Leaves | [d-1] | | kG\_LFGr | | 0.035 | [6] | |
| Biotransformation rate constants: |  | |  | |  |  | |
| Roots | [d-1] | | kM\_RGr | | Chemical dependent |  | |
| Leaves | [d-1] | | KM\_LFGr | | Chemical dependent |  | |

data are defined for the plane of the leaf surface ALF\_Gr (Table 6), [19,48]. The experimental data did not distinguish between cuticular and stomatal pathways of exposure, but since only hydrophobic organic compounds were included in the measurements and the stomatal exchange can be assumed to be negligible for these kinds of compounds, it can be assumed that the obtained mass transfer coefficients refer to the cuticular exchange only.

Adopting the approach presented in [6], the mass transfer coefficient for the stomatal gaseous exchange k’stom\_Gr (m d-1) is calculated by applying Fick’s Law and adjusting the conductance of the stomatal pathway for the chemical, i.e. the mass transfer coefficient, to that for water vapour (which is passing through the stomata during transpiration). It is defined as a function of temperature, relative humidity, and the chemicals molecular weight (Table 6).

The particle bound deposition includes both wet and dry deposition. Its mass transfer coefficient k’p\_Gr is parameterized based on measurements of deposition to the plane of the canopy (AC\_Gr) of pasture land in Germany [46] (Table 6). The corresponding D values for the different pathways of atmospheric deposition are given in Table 4.

*Biotransformation.* Biotransformation including both the abiotic and biotic degradation processes is described as a first order reaction process. It is defined independently for the leaf and the root compartment. The rate constants kM\_LFGr and kM\_RGr with units of (d-1) are chemical specific and user defined.

*Growth as pseudo-elimination pathway.* On the premise of exponential growth, chemical dilution in the plant compartments due to growth can be described with a pseudo-loss D value (see e.g. [8,50]; Table 4). The growth rate constants for the root compartment kG\_RGr and the leaf compartment kG\_LFGr with units of (d-1) are given in Table 6.

### Cultivated plants

Four types of cultivated plants are considered in the model: aerial fruits (including fruit, vegetable and grain, identifier v1), subterraneous tubers (identifier v2), leafy vegetable (v3), and root fruits (v4). The exposure of the cultivated plants to organic chemicals is described with a three-compartment model distinguishing between a root, a leaf, and a fruit compartment following the approach presented in [20]. The model is based on the grass model described above, which has been extended by a fruit compartment. The processes for chemical uptake and elimination considered in the model are the transport with the phloem flow from the leaf to the fruit compartment (PhFR), advective transport with a fraction of the xylem flow which is branched off before entering the leaf compartment (trFR; only considered for aerial fruits), diffusive exchange with the ambient medium (Ga for aerial fruits v1; WT for tubers v2), biotransformation (M), and growth (G). The fugacity in the leaf compartment is hence calculated by extending equation 16 with an additional D value for the phloem flow into the fruit DphF\_v1,2 and, in the case of aerial fruits, subdividing the D value for the transport with the transpiration stream (Dtr) into one entering the leaf compartment (DtrLF\_v1) and one entering the fruit compartment (Dtr\_FR\_v1):

 (22)

The chemical fugacity in the fruit compartment is accordantly:

 (23)

 (24)

The index v1,2 stands for vegetation 1 with an aerial fruit compartment and vegetation 2 with a subterraneous fruit / tuber compartment. The indices Fr and phFR stand for the fruit compartment and the phloem stream from the leaf to the fruit compartment. In the case of leafy vegetables or root fruits, the volume of the fruit compartment is set to zero. Since the phloem flow rate into the fruit is defined as a function of the fruit surface area (see below; Table 7), this is tantamount to decoupling the fruit compartment, but leaves the user the possibility to individually parameterize the cultivated plants of interest. The equations for the D values are given in Table 4.

Plant leaves, aerial fruits, root fruits and tubers are described as a homogeneous mixture of lipids, proteins, and carbohydrates, air, and water in accordance with [20] (Table 3). For aerial fruits and leaves, lipids are modelled as 1-octanol (i.e. Klip = KOW) and the Z-values for proteins and carbohydrates are derived from the protein-water partition coefficient Kprot (m3 m-3) and the carbohydrate-water partition coefficient KCHO (L kg-1), both defined as a function of KOW [20,47] (Table 6). Note that different functions are used to calculate KProt and KCHO in roots and fruits.

Following the approach presented in [41] for potato and carrot, the lipids of the roots and tubers are modeled as *a*K OW(T)b where *b*, an empirical value describing differences between root lipids and *n*-octanol, is set to 0.77and *a* is 1.22.

The fruit Z values ZF\_v1,2  are hence in analogy to equation 20:

 (25)

where ρCHO is the density of carbohydrates (106 g m-3).

*Stem.* The stem is not considered in the model as an edible part of the plant. Depending on the kind of plant, the stem might, however, serve as an additional storage compartment causing an additional retention of in particular rather hydrophobic chemicals in their transfer to the leaves and aerial fruits. As for the roots, it can be assumed that the diffusive chemical uptake over the stem surface has a minor impact on the total chemical load reaching the edible parts of the plant; rather hydrophobic chemicals remain in the outer layer of the stem and do not reach the transpiration stream [51], whereas the advection with the transpiration stream dominates as transport process for the more hydrophilic compounds. For volatile compounds, finally, equilibrium partitioning is rapidly established between the leaves and the atmosphere [52], so that the possible contribution of the diffusive uptake into the stem and subsequent translocation into the leaf compartment to the chemical load in the leaves is cancelled out immediately. Consequently, the stem is not considered as a separate compartment in the model. To account though for the additional storage compartment and potential for chemical retention, the mass of the stem consisting of air, water, lipids, carbohydrates, and proteins can optionally be added to the mass of the root compartment under the assumption that the stem has the same growth rate and biotransformation rate as the root compartment.

*Root.* The root uptake is defined analogously to the grass module, considering the advective chemical uptake with the transpiration stream and subsequent establishment of an equilibrium partitioning between the transpiration stream and the root compartment (see above). In general, the biomasses of the root compartment MR and the leaf compartment MLF are assumed to be equal, as well as the respective growth rates. If the stem is assumed to contribute significantly to the chemical retention in the chemical transfer from the root to the leaf compartment, the stem biomass is added to the root biomass. MR an MLF are converted into the corresponding volumes VR an VLF (m3) by dividing by the root and leaf densities [20].

*Gaseous deposition.* In analogy to the grass module, both the gaseous exchange through the cuticle and through the stomata is considered as exposure pathway of leaves and fruits. Comparing field and laboratory data on mass transfer coefficients for the diffusion through the air-side and plant-side boundary layer of cuticles of rye grass [46] with calculated values using correlations with the chemicals’ properties as has been suggested in e.g. [53] suggests that the existing approximations have a tendency for overestimation, in particular for hydrophobic non-volatile compounds. As a consequence, for any plant species, the gaseous exchange through the cuticle is defined identical to the grass module by adopting the mass transfer coefficients obtained for the exposure of rye grass to hydrophobic organic compounds [19,46,48], (Table 7). To our knowledge, there are no data on the gaseous deposition to fruits available which could be generalized. The most reasonable approximation is to assume that the fruit cuticle has similar composition and properties as the leaf cuticle and that the same mass transfer coefficients can be applied (Table 7).

**Table 7.** Parameterization of the module for cultivated plants.

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | | | **Unit** | | | | **symbol** | | | **value / equation** | | | | **Ref.** | | | |
| Canopy area | | | [m2] | | ACP\_vx | | | | | 1 | | |  | | | | |
| Gaseous deposition (leaf and aerial fruit): | | | |  | | |  | | |  | | | |  | | | |
| Stomatal mass transfer coefficient | [m d-1] | | | | | k’stom\_vx | | | | | where MW is the chemical’s molecular mass (mol g-1), rh is the rel. humidity (set to 0.5), and T is the ambient temperature in (K) | | | | [6] | | |
| Gaseous deposition (leaf and aerial fruit): | | | |  | | |  | | |  | | | |  | | | |
| air-side mass transfer coefficient | | | [m m-2CP d-1] | | | k’gg\_vx | | | | 192 | | [46] | | | |
| plant-side mass transfer coefficient | | | [m m-2LF d-1] | | | k’gp\_vx | | | | 6.72∙10-7 | | | [19,48] | | | |
| Particle bound deposition (leaf and aerial fruit): | | | | | |  | |  | |  | | | |  | | | |
| Deposition velocity (wet & dry) | | | [m m-2CP d-1] | | | k’p\_vx | | | | 72 | | | [46] | | | |
| Fruit /Tuber– general parameters: | | |  | | |  | | | |  | | |  | | | |
| Soil water – tuber mass transfer coefficient | | | [m d-1] | | | k’WT\_v2 | | | |  | | | [6,41] | | | |
| Transpiration stream into fruit | | [m3 m-2LF d-1] | | | | GtrFR\_vx | | | |  | | | | | | |
| Transpiration stream into leaves | | [m3 m-2LF d-1] | | | | GtrLF\_vx | | | |  | | | | | | |
| Phloem flow rate into fruit | | [m3 m-2LF d-1] | | | | GphFR\_vx | | |  | | | | [6] | | | |

**Table 7 (continued).**

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | | **Unit** | **symbol** |  | | | | | | | | | | **Ref.** | |
| Fruit area | | [m2 m-3FR] | AFR\_vx |  | | | | | | | | | | [20] | |
| Root – general parameters: | |  |  |  | | | | | | | | | |  | |
| Density | | [g m-3] | ρroot/leaf\_vx | 9∙105 | | | | | | | | | | [20] | |
|  | |  |  | **Apple (v1)** | **Grain (v1)** | | **Potato (v2)** | | **Lettuce (v3)** | | **Carrot (v4)** | | |  | |
| Leaf area | | [m2 m-3LF] | ALF\_vx | 4100 | 5000 | | 2000 | | 5000 | | 2000 | [6,13,20,21] | | | |
| Leaf volume | | [m3 m-2CP] | VLF\_vx | 4.9∙10-4 | 2.2∙10-3 | | 1∙10-3 | | 2.2∙10-3 | | 1∙10-3 | | |  | |
| Leaf growth rate constant | | [d-1] | kG\_LFvx | 0.035 | 0.035 | | 0.035 | | 0.035 | | 0.035 | | | [6] | |
| Leaf biotransformation rate constant | | [d-1] | kM\_LFvx | 0 | 0 | | 0 | | 0 | | 0 | | |  | |
| Fruit & tuber volume | | [m3 m-2CP] | VFR\_vx | 5.35∙10-3 | 2.8∙10-4 | | 2∙10-3 | | — | | — | | | [6,21,54] | |
| Number fruits/tubers | | [m-2CP] | nFR | 20 | 7181 | 30 | | **—** | | **—** | | | [54,55] | |
| Fruit growth rate constant | | [d-1] | kG\_FRvx | 0.035 | 0.035 | | 0.139 | |  | |  | | | [6,21] | |
| Fruit ripening period | | [d] | tFR | 60 | 60 | | 60 | |  | | 60 | | |  | |
| Fruit biotransformation rate constant | | [d-1] | kM\_Rvx | 0 | 0 | | 0 | | 0 | | 0 | | |  | |
| Root volume | | [m3 m-2CP] | VR\_vx | 0.045 | 2.2∙10-3 | | 9.2∙10-4 | | 2.2∙10-3 | | 0.031 | | | [56] | |
| Root growth rate constant | | [d-1] | kG\_Rvx | 0.1 | 0.035 | | 0.035 | | 0.035 | | 0.1 | | | [7,21] | |
| Root biotransformation rate constant | | [d-1] | KM\_Rvx | 0 | 0 | | 0 | | 0 | | 0 | | |  | |
| Transpiration rate | [m3 d-1 m-2LF/FR] | | Gtr\_vx | 6∙10-4 | 4.8∙10-4 | | 2∙10-4 | | 4.8∙10-4 | | 2∙10-4 | | | [20,57,58] | |

In analogy to the grass module, the mass transfer coefficient for stomatal gaseous exchange k’stom\_vx (m d-1) is defined adopting the approach from Trapp [6], i.e. applying Fick’s Law and adjusting the mass transfer coefficient for the chemical’s stomatal pathway to the one for water vapour. It is defined as a function of temperature, relative humidity, and the chemical’s molecular weight [6], (Table 7).

*Particle bound deposition.* For the particle bound deposition mass transfer coefficient k’p\_vx (m d-1), the value from the grass model of 72 m d-1 is adopted [46]. Note that this value is defined for the plane of the canopy.

*Biotransformation.* Biotransformation, which includes both abiotic and biotic degradation processes, is described as a first order reaction process. It is defined independently for the leaf, fruit, and the root compartments. The rate constants kM\_LFvx with units of (d-1) are chemical specific and user defined.

*Crop type specific characteristics.*

*v1 – aerial fruits*. In this context, the term aerial fruit is used synonymously for aerial fruits, (non-leafy) vegetables, and grains. Chemical uptake and elimination pathways considered for the fruit compartment are the advective transport into the compartment with the phloem and a fraction of the xylem flow, as well as diffusive exchange with the atmosphere through stomata and the cuticle.

The fraction of the transpiration stream diverging from the main stream and getting directly into the fruit compartment GtrFR\_vx is assumed to be proportional to the ratio of the amount of fruit stomata to the total number of stomata in fruits and leaves [20]. The ratio is calculated on the basis of the fruit and leaf areas.

Assuming that the entire dry weight content of the fruit originates from the phloem, the phloem flow rate from the leaf into the fruit GphFR\_vx in m3 d-1 is estimated on the basis of the dry weight contents of the fruit and of the phloem sap, and the fruit’s ripening period [6], Table 7.

Apples and grains are set as default representatives for aerial fruits (Table 7). In case of the apple tree, the stem volume is added to the root compartment. The cereal leaf and root compartment were parameterized adopting the parameterization of the grass (Table 7).

*v2 – subterraneous tubers*. Subterraneous fruits are tubers, i.e. in contrast to root fruits, they are not part of the root system for water uptake. They are modelled similar to the aerial fruits with a connection to the leaf compartment via the phloem flow. However, there is no direct link from the root compartment to the tuber via the transpiration stream. Diffusive exchange with the surrounding soil is described with the effective chemical diffusivity in potato tissue, applying the model approach suggested in [41]. The resulting mass transfer coefficient k’WT\_v2 (m h-1) is given in Table 7. The phloem flow rate is calculated in the same way as for aerial fruits (see above).

Potatoes are set as default representatives for subterraneous tubers (Table 7). Due to the generally lower leaf area index of potatoes compared to e.g. lettuce or grass, a default value of 2000 m2 m-3 leaf area was applied; the root volume and the transpiration stream were reduced accordingly.

*v3 – leafy vegetables*. Lettuce was chosen as default representative for leafy vegetables (Table 7). The fruit volume and thus the phloem flow into the fruit compartment is set to zero for this type of vegetables. For the root compartment, the parameterization of the grass was adopted; the leaf compartment was parameterized based on the data given in [20], (Table 7).

*v4 – root fruits*. Carrots were chosen as default representatives for root fruits (Table 7). The fruit volume, and thus the phloem flow into the fruit compartment is set to zero for this type of vegetable in the same way as for leafy vegetables. The leaf compartment was parameterized in the same way as for potatoes; for the root compartment, the additional mass of the root fruits was considered.

### Cattle

The bioaccumulation model for milk cows and beef cattle is adopted from [13]. In the original model a steady-state approach was applied for milk cows on the basis of the work from [59], whereas bioaccumulation in beef cattle was described with a non-steady state approach. In this model, also the latter has been translated into a steady-state model, assuming that the high pseudo-elimination of contaminants due to the rapid growth of domestic beef cattle has a similar impact on the final concentrations in the beef tissue as the loss with the daily lactation in milk cows. Similar to the human, the cattle is described with a two-compartment model which distinguishes between the gastrointestinal tract and the body itself. The model considers chemical uptake with the inhaled air as well as with ingested fodder, soil, and water, and chemical elimination with the exhaled air, feces, urine, metabolism, as well as lactation in the case of milk cows and growth in the case of beef cattle. Applying equation yields for the chemical fugacity in milk cows and in the cow’s milk fMC:

 (26)

and for the chemical fugacity in beef cattle fBC:

 (27)

The indices C, MC and B stand for cattle in general, milk cow and beef cattle, respectively. Ui, re, gb, L, M, ur, and G stand for ingestion of fodder i, respiration, gastrointestinal-body transfer, lactation, metabolism, urination, and growth. EOC is the dietary absorption efficiency estimated in accordance with [13,59]. The bi-directional transfer across the digestive tract membrane Dgb\_C is described using the two-film concept with a water and a lipid resistance as described in [59]. Otherwise, the same approaches for the description of the uptake and elimination processes as for the human module are applied. The D-values are defined in Table 4; the parameterization of the model is given in Table 8. The fugacity capacities of the milk cow, beef cattle and cow milk are defined by applying equation 7 and using the weight fractions and densities listed in Table 3. The body mass of the milk cow MC is set to 600 kg, the mass of the beef cattle MMC is set to 700 kg.

*Food composition.* In addition to grass as main fodder and vector of exposure to organic chemicals, the model takes into account that cattle eat a substantial amount of soil while grazing [60]. Contamination from other feed than grass is assumed to be about 25% of the total contamination load taken up with the fodder [61].

*Growth as pseudo-elimination pathway.* On the premise of exponential growth, chemical dilution in the organism due to the organisms’ growth can be described with a pseudo-loss D value (see e.g. [8,50]; Table 4). Beef cattle growth rate constant was estimated through comparing BMFs generated by ACC-HUMAN (dynamic, 28 month simulation) to ACC-HUMANsteady (no growth) across a range of physical-chemical properties. The growth dilution rate for a 700 kg animal that results in similar values was determined.  The underlying reason for determining a growth rate through this approach is that it is necessary to account for the rapid growth (and hence tendency to dilute chemical concentrations) experienced by the cow over the 28-month life span. The growth rate constant of 0.03 (d-1) is adopted. Note that growth is only considered in beef cattle; milk cows are assumed to be full-grown.

**Table 8.** Default parameterization of the cattle module in accordance with [13].

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
|  | **Unit** | | **symbol** | **value / equation** | | | **Ref.** |
| **Beef cattle** | **Milk cow** | |
| Ingestion rates: |  | |  |  |  | |  |
| grass | [kgdw d-1] | |  | 19 | 13 | | [62] |
|  | [mfw3 d-1] | | GUG\_BC/MC | 0.09 | 0.065 | |  |
| soil | [g d-1] | |  | 440 | 300 | | [62] |
|  | [m3 d-1] | | GUS\_BC/MC | 2.59∙10-4 | 1.76∙10-4 | |  |
| water | [m3 d-1] | | GUW\_BC/MC | 0.05 | 0.07 | |  |
| Contribution of grass to total dietary exposure |  | GrExp\_BC/MC | | 0.75 | 0.75 | | [61] |
| Absorption efficiency |  | |  |  | | | [59,63] |
| Respiration rate | [m3 d-1] | | Gre\_BC/MC | 150 | 150 | | [13] |
| Urination rate | [m3 d-1] | | Gur\_BC/MC | 0.05 | 0.05 | | [13] |
| Metabolism rate constant |  | | kM\_BC/MC | Chemical specific | | |  |
| Lactation rate | [m3 d-1] | | GL\_ MC | — | 0.017 | | [59] |
| Growth rate constant \* | [d-1] | | kG\_BC/MC | 0.03 | | 0 |  |
|  | | | | | | | |

## Aquatic Food Chain

### Zooplankton.

Equilibrium partitioning between zooplankton and water is assumed following the approach presented in [13] and supported by recent field and laboratory data [64,65].

 (28)

In order to ensure the applicability to a large range of chemicals, both lipids (indicator: lip), NLOM, and water (W) are considered as sorbing matrices in zooplankton in accordance with [15,66]. The sorption capacity Zzoo is calculated with equation 7. The volume fractions of lipids, NLOM, and water (*v*lip\_zoo, *v*NLOM\_zoo, and *v*W\_zoo, respectively) are given in Table 3.

### Benthos.

Benthic organisms constitute an important link in the uptake of organic contaminant into aquatic food webs and hence the wildlife exposure to these compounds. In order to cover a broad range of prey organism for the aquatic organisms on higher trophic levels, three types of benthic invertebrates are considered in the aquatic food web module with different trophic positions and feeding strategies (i.e. vectors of exposure). For the first trophic level, an invertebrate (b1) with similar bioaccumulation behaviour as the bulk zooplankton and serving primarily as prey item for a benthic predator is described, as well as a filter feeder (b2). The third benthic invertebrate is designed in a way that it can be parameterized as a deposit feeder and/or a predator. The model descriptions for chemical bioaccumulation in benthic organisms is based on [14,15,67]. The sorbing matrix for all invertebrates is assumed to consist of lipids, NLOM, and water [15,66], and the Z values Zbx (where *bx* stands for benthic invertebrate b1, b2 and b3, respectively) is calculated according to equation 7. The volume fractions of lipids, NLOM, and water (*v*lip\_bx, *v*NLOM\_bx, and *v*W\_bx, respectively) are given in Table 3.

*Invertebrate b1*. The invertebrate b1 can be viewed as a small amphipod spending a given time period in the sediment (expressed as time fraction TFS (h h-1)) and the remaining time of the day in the overlaying water (expressed as time fraction TFW (h h-1)). As for the zooplankton, chemical equilibrium partitioning with the surrounding medium is assumed, in which b1 is assigned a chemical fugacity equal to the weighted mean fugacity of sediment and water on the basis of the time daily spent in water and sediment:

 (29)

The default parameterization is based on field data from the amphipods *Monoporeia affinis* and *Diporeia affinis* [3,68-70]; TFS and TFW were set to 0.9 and 0.1, respectively [70].

*Invertebrates b2 & b3*. Comparable modelling approaches on the basis of [14,15,67] are applied to describe bioaccumulation in the filter feeder b2 and the deposit feeder/predator b3. Uptake and elimination processes considered are the diffusive chemical exchange with the porewater and the water overlaying the upper sediment layer via respiratory surfaces, chemical uptake with food, and loss due to metabolism, egestion and growth. The major difference between the model descriptions of the two benthic invertebrates is the process description of contaminant uptake with diet. Applying equation gives for the fugacity at steady state:

 (30)

 (31)

where the indices *U*, *b1, SS, S, O, P,* *V*, *E*, *M*, and *G* stand for food, benthic invertebrate b1 (i.e. prey), suspended material, sediment, water overlaying the sediment, porewater, gill ventilation, egestion, metabolism and growth, respectively. E0\_b is the gut absorption efficiency. The fugacity of the respired water is approximated as a weighted mean value of the fugacities of the overlaying water and the porewater; VF stands for the volume fraction of the respective respired water. Adopting the approximation suggested in [15], 95% of the respired water were assumed to originate from the layer overlaying the sediment, and the remaining 5% from sediment porewater. The equations for the D values are given in Table 4. The volume fractions of the different phases building up the sorbing matrix of filter feeders given in Table 3 were compiled from data on blue mussel (*Mytilus edulis*) [25], those for the deposit feeder/ predator from data on the isopod *Saduria entomon* (*Mesidotea entomon*) [26,27].

*Gill ventilation.* Contaminant uptake and elimination via gill ventilation can be described as a diffusive process, which implies that the D values for uptake and elimination are equal. The uptake rate constant k1 (L kg-1 d-1) is defined as a function of the fish mass MF1,2 (kg) and the chemical’s KOW in accordance with [13,71,72].

*Ingestion.* Chemicaluptake with food is a combined process of ingestion (i.e. an advective contaminant transport into the gastrointestinal tract with the diet) and subsequent absorption (i.e. diffusive uptake across the intestinal wall). The ingestion D value for a given food item i is the product of the feeding rate GUi (m3 d-1), the Z value of the food item i ZUi, and the chemicals absorption efficiency E0\_biota (Table 4). For the filter feeder b2, the feeding rate GU\_b2 is described as the product of the gill ventilation rate, the particle fraction in the infiltrated water *v*SS [m3 m-3] (Table 1), and the filter feeder’s scavenging efficiency σb2 (Table 9), [14]. For the benthic invertebrate b3, the feeding rate is approximated with an allometric regression as suggested in [50], (Table 9).The default food composition was defined in line with food web interactions of the Baltic Sea (Table 11) [73].

**Table 9.** Parameterization of the benthic food chain.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | **unit** | **symbol** | **value / equation** | **Ref.** |
| Body mass |  |  |  |  |
| b2 (filter feeder) | [kg] | Mb2 | 1∙10-3 | [74] |
| b3 (predator) | [kg] | Mb3 | 7∙10-3 | [75] |
| Biota density | [g m-3] | ρb1,2,3 | 106 |  |
| Growth rate constant | [d-1] | kG\_b2,3 |  | [76] |
| Metabolism rate constant |  | kM\_b2,3 | chemical specific |  |
|  |  |  |  | [15] |
|  |  |  |  |  |
|  |  |  |  | [15] |
| Ventilation uptake rate constant | [L kg-1 d-1] | k1\_b2 |  | [13,71,72] |
| Ingestion rate b2 (filter feeder) | [m3 d-1] | GU\_b2 |  | [14] |
| Particle scavenging efficiency | [m3 m-3] | σb2 | 1 | [14] |
| Ingestion rate b3 (predator) | [m3 d-1] | GU\_b2 | where T is the ambient water temperature (K) | [50] |

**Table 9 (continued).**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | **unit** | **symbol** | **value / equation** | **Ref.** |
| gut absorption efficiency |  | E0b |  | [13,67,77,78] |
| Lipid assimilation efficiency |  | εlip | 0.75 | [15] |
| NLOM assimilation efficiency |  | εNLOM | 0.75 | [15] |
| Organic carbon assimilation efficiency |  | εOC | 0.46 | [14] |
| Water assimilation efficiency |  | εW | 0.25 | [15] |
| Egestion factor of b2 (filter feeder) |  | Qb2 |  | [14,15] |
| Egestion factor of b3 (filter feeder) |  | Qb3 | where | [14,15] |

**Table 10.** Parameterization of the fish module.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | **unit** | **symbol** | **value / equation** | **Ref.** |
| Body mass |  |  |  |  |
| F1 (planktivore) | [kg] | MF1 | 0.005 |  |
| F2 (piscivore) | [kg] | MF2 | 0.1 |  |
| Biota density | [g m-3] | ρF | 106 |  |
|  |  |  |  |  |
| Ventilation uptake rate constant | [L kg-1 d-1] | k1\_F1,2 |  | [13,71,72] |
| Ingestion rate | [m3 d-1] | GU\_F1,2 | where T is the ambient water temperature (K) | [50] |
| Density of prey | [g m-3] | ρprey\_F | 106 |  |
| gut absorption efficiency |  | E0\_F |  | [13,67,77,78] |
| Egestion factor |  | QF | 8 | [66] |
| Metabolism rate constant |  | kM\_F1,2 | Chemical specific |  |
| Growth rate constant | [d-1] | kG\_F1,2 |  | [76] |

Applying the two-film theory for the diffusive contaminant uptake from the gut through the gastrointestinal tract, the absorption efficiency E0b is defined as a function of KOW adopting the correlation for fish suggested in [13] on the basis of data from [67,77,78] (Table 9).

*Egestion.* The decrease of the sorption capacity of the ingested food as a result of the digestion process is characterized by the egestion factor Qb, which corresponds to the ratio of the D values for ingestion and egestion. Assuming that the efficiency of chemical transfer over the gut membrane is equal in both directions, Qb2,3 can be expressed as the quotient of the organism-water partition coefficient KbxW and the feces-water partition coefficient KFW\_bx. Applying the approach suggested in [14,15] and expressing KF\_bxW as a function of the dietary assimilation efficiencies εi of the different components i of the diet (lip: lipids; NLOM: non-lipid organic matter; W: water; OC: organic carbon) yields equations 32 and 33 for the filter feeder’s Qb2 and the deposit feeder’s/predator’s Qb3, respectively.

 (32)

 (33)

where the feces-water partition coefficient KFW\_b3 is:



*Growth.* The growth rate constant kG\_b2,3 with units in (d-1) is dependent on the species, weight and ambient water temperature. For the default setting, a generalized allometric relationship was applied as suggested in [76] for aquatic organisms (Table 9). The relationship yields predictions of the mass increase with time of both the filter feeder *Mytilus edulis* and the benthic predator *Saduria entomon* which are in good agreement with field data [27,75,79].

*Metabolism.* Metabolism is described as a first order reaction process. The metabolism rate kM\_b2,3 is chemical specific and user defined.

### Fish.

Two fish are included in the bioaccumulation model, allowing predictions of the chemical concentrations in planktivorous and piscivorous fish, both of which contribute to the human diet and thus the dietary exposure of humans to organic contaminants. Adopting the parameterization given in [13], Baltic herring and cod were chosen as representatives for the forage and predator fish. The difference between the two fish is the parameterization including the prey preferences as listed in Table 11; the same modelling approach is applied for both fish.

The fish bioaccumulation model is designed in accordance with [13,66]. Applying equation gives for the fish fugacity at steady state:

 (34)

where the indices *F,* *Ui*, *V*, *E*, *M*, and *G* stand for the fish, the (ingestion of) food item i, gill ventilation, egestion, metabolism and growth, respectively. Equations for the D values are given in Table 4. The Z value is calculated applying equation 7.

*Gill ventilation.* Contaminant uptake and elimination via gill ventilation is described as a diffusive process (Table 4). The uptake rate constant k1 (L kg-1 d-1) is defined as a function of the fish mass MF1,2 (kg) and the chemical’s KOW in accordance with [13,71,72], (Table 10).

*Ingestion.* Chemicaluptake with food is a combined process of ingestion (i.e. an advective contaminant transport into the gastrointestinal tract with the diet) and subsequent absorption (i.e. diffusive uptake across the intestinal wall). The D value for the ingestion is hence the product of the feeding rate GUi (m3 d-1), the weighted mean Z value of the prey ZUF1,2 (), and the chemicals absorption efficiency E0\_F (Table 4). For the approximationof the feeding rate, an allometric regression is applied as suggested in [50] (Table 10).

The default food composition is set in line with food web interactions of the Baltic Sea (Table 11) [73]. Applying the two-film theory for the diffusive contaminant uptake from the gut through the gastrointestinal tract, the absorption efficiency E0\_F is defined as a function of KOW [77,78], adopting the correlation suggested in [13] on the basis of data from [67,77,78] (Table 10).

*Egestion.* The decrease of the sorption capacity of the ingested food as a result of the digestion process is characterized by the egestion factor QF, which corresponds to the ratio of the D values for ingestion and egestion. As default, QF was assigned a value of 8 in accordance with data reported for rainbow trouts [66].

*Growth*The growth rate constant kGF with units of (d-1) is defined based on allometric relationship suggested in [76].

*Metabolism.* Metabolism is described as a first order reaction process. The metabolism rate kM\_F1,2 is chemical specific and user defined.

**Table 11.** Feeding preferences. Mass fractions *y*prey i\_biota in (g g-1) of the different food items in the diet of the aquatic organisms.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| prey | predator |  |  |  |  |  |
|  | **Benthos 1** | **Benthos 2** | **Benthos 3** | **Fish 1** | **Fish 2** | **Seal** |
| Suspended matter |  | 0.5 |  |  |  |  |
| Sediment | 1 | 0.5 | 0.7 |  |  |  |
| Zooplankton |  |  |  | 1 |  |  |
| Benthos 1 |  |  | 0.3 |  | 0.05 |  |
| Benthos 2 (filter feeder) |  |  |  |  | 0.05 | 0.001 |
| Benthos 3 (pred. & dep. feeder) |  |  |  |  | 0.4 | 0.007 |
| Fish 1 |  |  |  |  | 0.5 | 0.916 |
| Fish 2 |  |  |  |  |  | 0.076 |

# Literature Cited

1. Morrison HA, Gobas F, Lazar R, Haffner GD. 1996. Development and verification of a bioaccumulation model for organic contaminants in benthic invertebrates. *Environmental Science & Technology* 30:3377-3384.

2. Campfens J, Mackay D. 1997. Fugacity-Based Model of PCB Bioaccumulation in Complex Aquatic Food Webs. *Environmental Science & Technology* 31:577-583.

3. Morrison HA, Whittle DM, Metcalfe CD, Niimi AJ. 1999. Application of a food web bioaccumulation model for the prediction of polychlorinated biphenyl, dioxin, and furan congener concentrations in Lake Ontario aquatic biota. *Canadian Journal of Fisheries and Aquatic Sciences* 56:1389-1400.

4. Fraser AJ, Burkow IC, Wolkers H, Mackay D. 2002. Modeling biomagnification and metabolism of contaminants in harp seals of the Barents Sea. *Environmental Toxicology and Chemistry* 21:55-61.

5. Cousins IT, Mackay D. 2001. Strategies for including vegetation compartments in multimedia models. *Chemosphere* 44:643-654.

6. Trapp S. 2007. Fruit Tree model for uptake of organic compounds from soil and air. *SAR and QSAR in Environmental Research* 18:367-387.

7. Trapp S. 2002. Dynamic root uptake model for neutral lipophilic organics. *Environmental Toxicology and Chemistry* 21:203-206.

8. Mackay D. 2001. *Multimedia environmental models, the fugacity approach*. Lewis, Boca Raton, FL, USA.

9. EC. European Union System for the Evaluation of Substances 2.0 (EUSES 2.0). Prepared for the European Chemicals Bureau by the National Institute of Public Health and the Environment (RIVM). 2004. Bilthoven, The Netherlands.

10. EC European Commission. Technical Guidance Document in support of Commission Directive 93/67/EEC on Risk Assessment for new notified substances, Commission Regulation (EC) No 1488/94 on Risk Assessment for existing substances and Directive 98/8/EC of the European Parliament and of the Council concerning the placing of biocidal products on the market. 2008.

11. Sabljic A, Gusten H, Verhaar H, Hermens J. 1995. Qsar modeling of soil sorption - improvements and systematics of log K-Oc vs log K-Ow correlations. *Chemosphere* 31:4489-4514.

12. Wania F, Daly GL. 2002. Estimating the contribution of degradation in air and deposition to the deep sea to the global loss of PCBs. *Atmospheric Environment* 36:5581-5593.

13. Czub G, McLachlan MS. 2004. A food chain model to predict the levels of lipophilic organic contaminants in humans. *Environmental Toxicology and Chemistry* 23:2356-2366.

14. Morrison HA, Gobas FAPC, Lazar R, Haffner GD. 1996. Development and verification of a bioaccumulation model for organic contaminants in benthic invertebrates. *Environmental Science and Technology* 30:3377-3384.

15. Arnot JA, Gobas FAPC. 2004. A food web bioaccumulation model for organic chemicals in aquatic ecosystems. *Environmental Toxicology and Chemistry* 23:2343-2355.

16. ICRP. 2003. *International Commission on Radiological Protection.*

*Basic anatomical and physiological data for use in radiological*

*protection: reference values. ICRP Publication 89*. Pergamon Press, Oxford.

17. USDA United States Department of Agriculture. National Nutrient Database for Standard Reference. http://www.nal.usda.gov/fnic/foodcomp/search/ . 2008.

18. Riederer M. 1990. Estimating partitioning and transport of organic-chemicals in the foliage Atmosphere system - discussion of a fugacity-based model. *Environmental Science & Technology* 24:829-837.

19. Tolls J, McLachlan MS. 1994. Partitioning of semivolatile organic compounds between air and Lolium multiflorum (Welsh ray grass). *Environmental Science and Technology* 28:159-166.

20. Undeman E, Czub G, McLachlan MS. 2009. Addressing temporal variability when modeling bioaccumulation in plants. *Environmental Science & Technology* 43:3751-3756.

21. Legind CN, Trapp S. 2009. Modeling the exposure of children and adults via diet to chemicals in the environment with crop-specific models. *Environmental Pollution* 157:778-785.

22. Trapp S. 1995. Model for uptake of xenobiotics into plants. In Trapp S, Mc Farlane C, eds, *Plant Contamination: modeling and simulation of organic chemical processes*, Plant Contam. Lewis Publishers, pp 107-153.

23. McLachlan, M. S. Slaughter weight of cattle; unpublished data. 2008. Personal Communication

24. McLachlan MS. 1993. Mass Balance of Polychlorinated-Biphenyls and Other Organochlorine Compounds in A Lactating Cow. *Journal of Agricultural and Food Chemistry* 41:474-480.

25. Vareltzis P, Undeland I. 2008. Removal of lipids and diarrhetic shellfish poisoning toxins from blue mussels (Mytilus edulis) during acid and alkaline isolation of proteins. *Journal of Agricultural and Food Chemistry* 56:3675-3681.

26. Korczynski RE. 1989. Biochemical composition of the isopod Mesidotea entomon (Linnaeus) from the Western Arctic. *Polar Biology* 9:391-395.

27. Aljetlawi AA, Sparrevik E, Leonardsson K. 2004. Prey-predator size-dependent functional response: derivation and rescaling the real world. *Journal of Animal Ecology* 73:239-252.

28. Schwalme K, Chouinard GA. 1999. Seasonal dynamics in feeding, organ weights, and reproductive maturation of Atlantic cod (Gadus morhua) in the southern Gulf of St Lawrence. *ICES Journal of Marine Science* 56:303-319.

29. Hoar WS, Randall DJ. 1969. *Fish physiology*. Academic press, New York.

30. Soengas JL, Strong EF, Fuentes J, Veira JAR, Andres MD. 1996. Food deprivation and refeeding in Atlantic salmon, Salmo salar: Effects on brain and liver carbohydrate and ketone bodies metabolism. *Fish Physiology and Biochemistry* 15:491-511.

31. Sarkar SR, Kuhlmann MK, Khilnani R, Zhu FS, Heymsfield SB, Kaysen GA, Levin NW. 2005. Assessment of body composition in long-term hemodialysis patients: Rationale and methodology. *Journal of Renal Nutrition* 15:152-158.

32. McLachlan MS, Czub G, Macleod M, Arnot JA. 2011. Bioaccumulation of organic contaminants in humans: a multimedia perspective and the importance of biotransformation. *Environ Sci Technol* 45:197-202.

33. van der Molen GW, Kooijman SALM, W. S. 1996. A Generic Toxicokinetic Model for Persistent Lipophilic Compounds in humans: An Application to TCDD. *Fundamental And Applied Toxicology* 31:83-94.

34. Moser GA, McLachlan MS. 2002. Modeling digestive tract absorption and desorption of lipophilic organic contaminants in humans. *Environmental Science & Technology* 36:3318-3325.

35. Deurenberg P, Weststrate JA, Seidell JC. 1991. Body-mass index as a measure of body fatness - age-specific and sex-specific prediction formulas. *British Journal of Nutrition* 65:105-114.

36. Barbieri HE, Pearson M, Becker W. Riksmaten - barn 2003. Livsmedels- och näringsintag bland barn i Sverige. Livsmedelsverket, Sweden.

37. Becker W, Pearson M. Riksmaten 1997-98. Kostvanor och näringsintag i Sverige. Metod- och resultatanalys. Livesmedelsverket, Sweden.

38. Hickie BE, Mackay D, de Koning J. 1999. Lifetime pharmacokinetik model for hydrophobic contaminants in marine mammals. *Environmental Toxicology and Chemistry* 18:2622-2633.

39. Geusau A, Tschachler E, Meixner M, Päpke O, Stingl G, McLachlan MS. 2001. Cutaneous elimination of 2,3,7,8-tetrachlorodibenzo-*p* -dioxin. *British Journal of Dermatology* 145:938-943.

40. McLachlan MS. 1996. Bioaccumulation of hydrophobic chemicals in agricultural food chains. *Environmental Science and Technology* 30:252-259.

41. Trapp S, Cammarano A, Capri E, Reichenberg F, Mayer P. 2007. Diffusion of PAH in potato and carrot slices and application for a potato model. *Environmental Science & Technology* 41:3103-3108.

42. Chiou CT, Sheng G, Manes M. 2001. A partition-limited model for the plant uptake of organic contaminants from soil and water. *Environmental Science and Technology* 35:1437-1444.

43. Koemp P, McLachlan MS. 1997. Interspecies variability of the plant/air partitioning of polychlorinated biphenyls. *Environmental Science and Technology* 31:2944-2948.

44. Koemp P, McLachlan MS. 1997. Influence of temperature on the plant/air partitioning of semivolatile organic compounds. *Environmental Science and Technology* 31:886-890.

45. Briggs G, Bromilow RH, Evans AA. 1982. Relationships between lipophilicity and root uptake and translocation of nonionized chemicals by barley. *Pesticide Science* 13:495-504.

46. Welsch-Pausch K. 1998. Atmosphärische deposition polychlorierter dibenzo-p-dioxine und dibenzofurane auf futterpflanzen. University of Bayreuth.Thesis

47. Debruyn Adrian MH, Gobas Frank APC. 2007. The sorptive capacity of animal protein. *Environ Toxicol Chem* 26:1803-1808.

48. McLachlan MS, Welsch-Pausch K, Tolls J. 1995. Field validation of a model of the uptake of gaseous SOC in Lolium multiflorum (Welsh Ray Grass). *Environmental Science and Technology* 29:1998-2004.

49. Paterson S, Mackay D, McFarlane C. 1994. A model of organic chemical uptake by plants from soil and the atmosphere. *Environmental Science and Technology* 28:2259-2266.

50. Gobas FAPC. 1993. A model for predicting the bioaccumulation of hydrophobic organic chemicals in aquatic food-webs: application to Lake Ontario. *Ecological Modelling* 69:1-17.

51. Trapp S, Miglioranza KSB, Mosbk H. 2001. Sorption of lipophilic organic compounds to wood and implications for their environmental fate. *Environmental Science and Technology* 35:1561-1566.

52. McLachlan MS. 1999. Framework for the interpretation of measurements of SOCs in plants. *Environmental Science and Technology* 33:1799-1804.

53. Kerler F, Schoenherr J. 1988. Permeation of lipophilic chemicals across plant cuticles: prediction from partition coefficients and molar volumes. *Archives of Environmental Contamination and Toxicology* 17:7-12.

54. Mitchell RAC, Mitchell VJ, Lawlor DW. 2001. Response of wheat canopy CO2 and water gas-exchange to soil water content under ambient and elevated CO2. *Global Change Biology* 7:599-611.

55. Best S, Salazar F, Bastias R, Leon L. 2008. Crop load estimation model to optimize yield – quality ratio in apple orchards, Malus Domestica Borkh, Var. Royal Gala. *Journal of information technology in agriculture* 7:11-18.

56. Macinnis-Ng CMO, Fuentes S, O'Grady AP, Palmer AR, Taylor D, Whitley RJ, Yunusa I, Zeppel MJB, Eamus D. 2010. Root biomass distribution and soil properties of an open woodland on a duplex soil. *Plant and Soil* 327:377-388.

57. Backes M, Blanke MM. 2008. Water consumption and xylem flux of apple trees. *Acta Hort* 732:573-578.

58. Spanarkel, R and Drew, M. C. Germination and growth of lettuce (*Lactuca sativa*) at low atmospheric pressure. Physiologia plantarum 116, 468-477. 2002.

59. McLachlan MS. 1994. Model of the fate of hydrophobic contaminants in cows. *Environmental Science & Technology* 28:2407-2414.

60. Fries GF. 1996. Ingestion of sludge applied organic chemicals by animals. *Science of the Total Environment* 185:93-108.

61. McLachlan MS, Thoma H, Reissinger M, Hutzinger O. 1990. PCDD/F in an agricultural food chain. Part 1: PCDD/F mass balance of a lactating cow. *Chemosphere* 20:1013-1020.

62. McLachlan MS. 1997. A simple model to predict accumulation of PCDD/Fs in an agricultural food chain. *Chemosphere* 34:1263-1276.

63. McLachlan MS, Richter W. 1998. Uptake and transfer of PCDD/F by cattle fed naturally contaminated feedstuffs and feed contaminated as a result of sewage sludge application. Part I: Lactating cows. *Journal of Agricultural and Food Chemistry* 46:1166-1172.

64. Sobek A, Reigstad M, Gustafsson O. 2006. Partitioning of polychlorinated biphenyls between arctic seawater and size-fractionated zooplankton. *Environmental Toxicology and Chemistry* 25:1720-1728.

65. Sobek A, Cornelissen G, Tiselius P, Gustafsson O. 2006. Passive partitioning of polychlorinated biphenyls between seawater and zooplankton, a study comparing observed field distributions to equilibrium sorption experiments. *Environmental Science & Technology* 40:6703-6708.

66. Gobas FAPC, Wilcockson JB, Russell RW, Haffner GD. 1999. Mechanism of biomagnification in fish under laboratory and field conditions. *Environmental Science and Technology* 33:133-141.

67. Gobas FAPC, Muir DCG, Mackay D. 1988. Dynamics of dietary bioaccumulation and fecal elimination of hydrophobic organic-chemicals in fish. *Chemosphere* 17:943-962.

68. Van Bavel B, Naf C, Bergqvist PA, Broman D, Lundgren K, Papakosta O, Rolff C, Strandberg B, Zebuhr Y, Zook D, Rappe C. 1996. Levels of PCBs in the aquatic environment of the Gulf of Bothnia: Benthic species and sediments. *Marine Pollution Bulletin* 32:210-218.

69. Strandberg B, Bandh C, Van Bavel B, Bergqvist PA, Broman D, Ishaq R, Naf C, Rappe C. 2000. Organochlorine compounds in the Gulf of Bothnia: sediment and benthic species. *Chemosphere* 40:1205-1211.

70. Lindstrom M, Fortelius W. 2001. Swimming behaviour in Monoporeia affinis (Crustacea: Amphipoda) - dependence on temperature and population density. *Journal of Experimental Marine Biology and Ecology* 256:73-83.

71. Gobas F, Mackay D. 1987. Dynamics of hydrophobic organic chemical bioconcentration in fish. *Environmental Toxicology and Chemistry* 6:495-504.

72. Sijm DTHM, Verberne ME, Dejonge WJ, Part P, Opperhuizen A. 1995. Allometry in the uptake of hydrophobic chemicals determined in vivo and in isolated perfused gills. *Toxicology and Applied Pharmacology* 131:130-135.

73. Harvey CJ, Cox SP, Essington TE, Hansson S, Kitchell JF. 2003. An ecosystem model of food web and fisheries interactions in the Baltic Sea. *ICES Journal of Marine Science* 60:939-950.

74. Sukhotin AA, Abele D, Portner HO. 2002. Growth, metabolism and lipid peroxidation in Mytilus edulis: age and size effects. *Marine Ecology-Progress Series* 226:223-234.

75. Haahtela I. 1990. What do Baltic studies tell us about the isopod *Saduria entomon* (L..)? *Annales zoologici Fennici* **27**:269-278.

76. Gewurtz SB, Laposa R, Gandhi N, Christensen GN, Evenset A, Gregor D, Diamond ML. 2006. A comparison of contaminant dynamics in arctic and temperate fish: A modeling approach. *Chemosphere* 63:1328-1341.

77. Clark KE, Gobas FAPC, Mackay D. 1990. Model of organic chemical uptake and clearance by fish from food and water. *Environmental Science and Technology* 24:1203-1213.

78. Schenker U, MacLeod M, Scheringer M, Hungerbuehler K. 2005. Improving data quality for environmental fate models: a least-squares adjustment procedure for harmonizing physicochemical properties of organic compounds. *Environmental Science and Technology* 39:8434-8441.

79. Zotin AA, Ozernyuk ND. 2004. Growth characteristics of the common mussel Mytilus edulis from the White Sea. *Biology Bulletin* 31:377-381.