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Deliverable 3.2. - Overview of environmental factor influence over  
additive exposure and release into the environment

## **Deliverable of WP3**

### **D.3.2: Overview of environmental factor influence over additive exposure and release into the environment**

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## 1. Introduction

A chemical additive is a compound that generally remains in the final product. . It allows obtaining better product quality and also improving the production process and saving resources. Throughout of the RISKCYCLE project (coordination action, Grant Agreement number: 226552) the use of chemical additives in several industrial sectors (paper, leather, textile, lubricants and electronics) has been studied. These six selected sectors can be qualified as economic relevant in many developing and non-developing countries, generating lots of benefit from them. The outcome of this task carried out by the project consortium has been compiled in a book (to be published during the 2011) entitled “Global Risk-Based Management of chemical additives I: Production, usage and Environmental Occurrence” (Springer-Verlag, Handbook of Environmental Chemistry Series) which gather information about the use of chemical additives for the six industrial sectors, together with some representative worldwide case studies related to these sectors elaborated by experts in these topics.

A great concern exists regarding the environmental consequences associated to the large amount of chemical additives employed in the aforementioned sectors. Along the entire life cycle of the product (containing the additive) and particularly once it reaches the end of its useful life and becomes a waste, additives may be released to the environment leading to a risk for both the environment and the human health.

The present document is a revision about the factors affecting the chemical additives emissions and their main exposition routes. The Mackay fugacity model has been also presented, which relates the concentration of chemical additives in the different environmental compartments taking into account the physicochemical properties of each compound.

## **2. Overview of factors and properties affecting environmental release of chemicals**

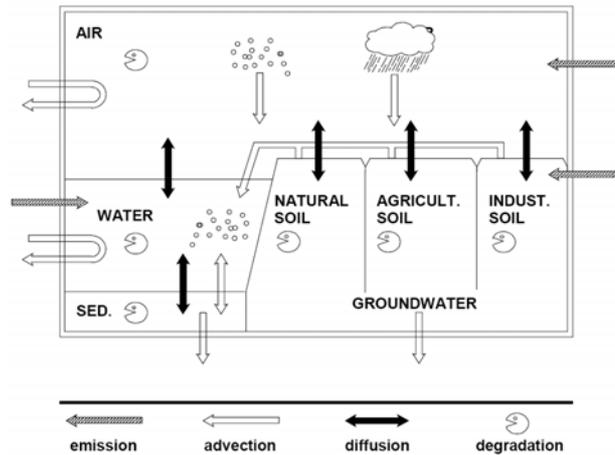
Information on the contaminant occurrence, fate and effects is important for managing ecosystem health, especially in heavily populated, industrial and/or agricultural regions where anthropogenic sources can be large and numerous. In principle, monitoring programs provide the most reliable means of quantifying contaminant concentrations. However, because of cost constraints for sampling and analysis, combined with temporal and spatial variability in large environmental scenarios, monitoring data may not always provide a reliable picture of exposure e.g., [1-3]. As an alternative to rely only on monitoring data, mass balance models have been successfully applied to predict contaminant fate in aquatic systems and thus they provide complementary information on environmental exposure and the risk of adverse effects. Provided that they have been properly evaluated, models can be used to estimate concentrations across a wide range of spatial and temporal scales and can also be used to explore scenarios, such as the potential impacts resulting from the release of new chemicals or from changes in the used quantity. Although data on chemical properties, chemical emission rates and the hydrology of receiving waters are usually required [4-7], these chemical-specific and system-specific data may be easier to obtain or estimate (e.g., from permanent in-stream flow gauges and per capita chemical usage estimates) than representative monitoring data.

Regional computations are done by means of multimedia fate models based on the fugacity concept; some of them have been described by [8-10]. These models are box models, consisting of a number of compartments which are considered homogeneous and well mixed. A substance released into the model scenario is distributed between the compartments according to the properties of both the substance and the model environment. Several types of fate processes are distinguished in the regional assessment, as drawn in Figure 1:

- Emission: direct and indirect to the compartments air, water, sediments, industrial soil and agricultural soil.
- Degradation: biotic and abiotic degradation processes in all compartments.

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- Diffusive transport: diffusive mass transfer between two compartments goes both ways. The net flow may be either way, depending on the concentration in both compartments.
- Advective transport (e.g. deposition, run-off, erosion): a substance is carried from one compartment into another by a carrier that physically flows from one compartment into the other. Therefore, advective transport is strictly one-way.



**Figure 1:** Relevant emission and distribution routes in environmental compartments  
([ECB: Technical guidance document on Risk Assessment, \[11\]](#))

In general, contamination levels tend to be higher when they are close to emission sources of a chemical and they decline with the increase of distance as a result of dilution, dispersion and degradation. However, this may be not always the case; circumstances have been described when contamination levels are higher further away from sources than at the sources themselves. Noticeable examples are the elevated levels of persistent, hydrophobic, organic chemicals found in the Arctic, in mountain regions and in forest soils [12]. Such long range transport of pollutants to remote areas may take place through a stepwise process known as *grasshopper effect*, based on the difference in the earth temperatures (Figure 2). This transport mechanism is common for persistent compounds, mainly those which are susceptible to volatilize. Temperature governs the global partitioning of semi-volatile air pollutants leading to a gradual accumulation of these compounds in the air of high latitudes. High quantities of persistent organic pollutants (POPs) are captured from the atmosphere by the vegetation in remote arctic regions and sub-arctic mountain ecosystems, which acts as important receptor of airborne xenobiotics.

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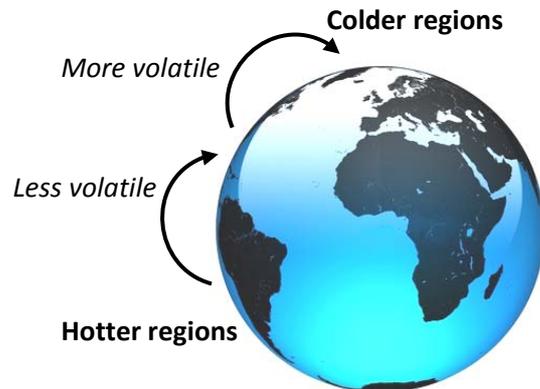


Figure 2: Long range transport of volatile POPs (“grasshopper effect”)

In summary, occurrence of pollutants in the environment may depend on three groups of factors, which are briefly discussed on the next sections:

- Intrinsic physical-chemical properties of the compound.
- Environmental (external) conditions.
- Anthropogenic factors.

## 2.1 Intrinsic physical-chemical properties

The behaviour patterns of a chemical compound (chemical additives in the RISKCYCLE framework) in the environment is strongly related to its physical-chemical properties. Therefore their knowledge is essential in order to model its distribution and fate within the different environmental compartments (soil, air, water, biota...). The most relevant are listed in Table 1.

**Table 1.** List of some physical-chemical properties relevant to the environmental fate of organic pollutants.

Property	Definition
<b>Atmospheric residence time (<math>\tau</math>)</b>	The ratio of the total mass of a chemical in an atmospheric compartment regarding the total emission rate or the total removal rate, under equilibrium conditions.
<b>Bioconcentration factor (BCF)</b>	The equilibrium ratio of the concentration of a chemical in an exposed organism to the concentration of the chemical in the surrounding habitat.
<b>Bioaccumulation potential</b>	The potential for an organism to absorb the chemical at a rate greater than that at which the substance is lost from the body.
<b>Biodegradation</b>	The transformation of chemical compounds by living organisms. Not confined to microorganisms (e.g., bacteria, fungi) but chiefly a microbial process in nature.
<b>Degradation temperature</b>	The temperature at which the given substance is no longer stable and begins to break down in its transformation products.
<b>Dry deposition</b>	Process by which atmospheric particles are transferred to the surface as a result of random turbulent air motions.
<b>Henry's Law constant (<math>H_c</math>)</b>	Describes the relative concentrations of a chemical in air (vapour phase) and the chemical dissolved in water, in a closed system at equilibrium. Henry's Law constant gives an indication of a chemical's tendency to volatilize from water to air or dissolve into water from air.
<b>Hydrolysis</b>	Chemical transformation process in which a chemical reacts with water. In the process, a new carbon-oxygen bond is formed with oxygen derived from the water molecule, and a bond is cleaved within the chemical between carbon and some functional group.
<b>Hydroxyl radical rate constant (<math>K_{OH}</math>)</b>	The rate constant for organic compounds photochemical reaction occurring in the atmosphere. New hydroxyl radicals are produced.
<b>Ionization or acid dissociation constant (<math>K_a</math>)</b>	An equilibrium ratio of the dissociation products and the parent compound in aqueous solutions. The degree of dissociation can alter the solubility and adsorption characteristics of the compound.

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<b>pKa)</b>	
<b>Mobility</b>	The tendency for a chemical to move in the environment (i.e., through soil with the percolation of water).
<b>Octanol-water partition coefficient (<math>K_{ow}</math>)</b>	The equilibrium ratio of a chemical's concentration in the octanol phase to its concentration in the aqueous phase of a two-phase octanol/water system, typically expressed in log units (log Kow or logP ). Kow provides an indication of a chemical's fat solubility (lipophilicity), its tendency to bioconcentrate in aquatic organisms, and to sorb to soil or sediment.
<b>Organic carbon partition coefficient</b>	The proportion of a chemical sorbed to the solid phase, at equilibrium in a two-phase, water/soil or water/sediment system expressed on an organic carbon basis. Chemicals with higher $K_{OC}$ values are more strongly sorbed and, therefore, tend to be less mobile in the environment.
<b>Ozone depletion potential (ODP)</b>	The relative amount of degradation to the <u>ozone layer</u> it can cause compared with the potential of chlorofluorocarbon-11 (CFC-11) which is assigned a <u>reference value</u> of 1.
<b>Persistence</b>	The ability of a chemical substance to remain in a particular environment in an unchanged form. Is directly related to the chemical compound degradation pathways.
<b>Plant Uptake</b>	The uptake of a chemical into plants is expressed in terms of a bioconcentration factor for vegetation (Bv), which is the ratio of the concentration in the plant tissue to the concentration in soil.
<b>Soil or sediment sorption coefficient (<math>K_d</math>)</b>	The equilibrium ratio between a chemical sorbed to the solid phase and in solution in a two-phase, soil/water or sediment/water system.
<b>Smog-forming potential</b>	The chemical reaction of hydrocarbons to produce atmospheric photochemical oxidants such as ozone and other by-products contributing to the formation of smog.
<b>Treatability</b>	The amenability of a chemical substance or waste stream to removal during waste water treatment, without adversely affecting the normal operation of the treatment plant.
<b>Vapour pressure</b>	The pressure at which a liquid is in equilibrium with its vapour at 25°C. It is a measure of the tendency of a compound to vaporize.
<b>Volatilization</b>	The transport process by which a chemical substance enters the atmosphere by evaporation from soil or water.
<b>Wet deposition</b>	Process by which <u>aerosol</u> particles collect or deposit themselves on solid surfaces, decreasing the concentration of the particles in the air.

## 2.2 Environmental Conditions

Any attempt to model the spatial occurrence and fate of chemicals in the environment will require an appropriate choice of external environmental factors (i.e., climate, landscape, matrix, biological), which have a definite influence on the behaviour of the chemicals considered. Table 2 summarizes some of the most relevant.

It is worth mentioning that the availability of spatial data sets has been greatly increased by the current progress achieved on remote sensing technologies [13-14].

**Table 2:** Summary of environmental factors affecting occurrence of chemicals

<b>Matrix composition</b>	<ul style="list-style-type: none"><li>- pH, CaCO<sub>3</sub>, cationic exchange capacity (CEC).</li><li>- Nutrient status (competitive species in soil solution).</li><li>- Organic matter content (total carbon and organic carbon content).</li><li>- Redox potential.</li><li>- Soil texture, porosity, bulk density.</li></ul>
<b>Biological processes</b>	<ul style="list-style-type: none"><li>- Biodegradability and its influences on organism's biological processes.</li><li>- Transformation products.</li></ul>
<b>Climate conditions</b>	<ul style="list-style-type: none"><li>- Temperature.</li><li>- Humidity.</li><li>- Wind speed.</li><li>- Solar radiation (photodegradation).</li><li>- Rainfall.</li><li>- Water flow</li><li>-Water column depth</li></ul>

### 2.3 Anthropogenic factors

The emission of a chemical substance to the environment may occur during all stages of their life-cycle, from production to disposal or recovery. Assessment of emission rates to each environmental compartment (air, soil, water, sediment) potentially exposed is thus required as input data for modelling.

The assessment procedure should in principle take into consideration the the aspects presented in the next table:

**Table 3:** Chemical compound mode of use and main emission routes to the environment, these two factors should be considered for design environmental fate models.

<b>Production</b>	<ul style="list-style-type: none"> <li>• Transport and storage</li> <li>• Formulation (blending and mixing of substances in preparations)</li> <li>• Industrial/Professional use (large scale use including processing (industry) and/or small scale use (trade))</li> <li>• Private or consumer use</li> <li>• Service life of articles</li> <li>• Waste disposal (including waste treatment, landfill and recovery)</li> </ul>
<b>Mode of use</b>	<b>Closed cycle:</b> Products used within a controlled process, they are steadily recycled in the system or processed as waste. Many industrial products such as surfactants, solvents, salts are used in closed cycle. As well as the synthesis intermediates and catalysts those are widely used in the pharmaceutical industry.
	<b>Spreading:</b> Compounds such as pesticides are present in extensive areas since they are spread out directly to the environment.
	<b>Chemical additives:</b> Aids that remain in the final product (textile, electronics, paper, leather, lubricants etc.), including compounds such as dyes, plasticizers, waterproof aids or antimicrobials. When this products reaches the end of its useful life (product becomes waste), these additives can be released to the environment.
<b>Quantity of use</b>	The exposure risk of a specific substance is not only related to its mode of use but it also is directly related to its production volume and use patterns.
<b>Emission characteristics</b>	<b>Point:</b> Compounds are emitted from localized sources, such as industrial effluents (or spills) or from wastewater treatment plants (WWTP) effluents.

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	<p><b>Diffuse:</b> Organic pollutants (PCBs, flame-retardants, pharmaceuticals, personal care products, steroid sex hormones, drugs, etc.) can be propagated through the aquatic environment once they are released from WWTP, through surface run-off (pesticides) or by air emissions (PAHs, volatile compounds, etc.). This type of contamination is highly influenced by atmospheric phenomena and water bodies' behaviour.</p>
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As a representative example of how these production factors can be handled and quantified, the modelling approach proposed by the JRC [15] in order to update the list of priority compounds associated to the Water Framework Directive (Directive 2000/60/EC, [16]) is shown below. It is based on a parallel assessment of amount produced and usage pattern:

$$\text{Annual usage} = \text{Amount used annually (tonnes)} * \text{use index} * \text{tonnage multiplier} \quad (1)$$

Annual usage is quantified through the combination of three parameters, namely the amount used (Tonnage), the mode of use and a correcting factor, scored as indicated in Tables 4, 5 and 6 respectively.

**Table 4** Exposure assessment scores (see equation 1 for calculations)

Exposure score	Annual use (tons)
1	0-1
2	1-10
3	10-100
4	100-1000
5	>1000

Any substance that did not meet the minimum data requirements for exposure assessment a risk score of zero was assigned, indicating insufficient information (the same criterion is used for the hazard assessment).

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**Table 5:** Criterion used to calculate the use *index*

<b>Use pattern</b>	<b>Use</b>
Controlled system (isolated intermediate)	<i>0.1</i>
Industrial (non-dispersive) use	<i>0.2</i>
Wide dispersive use (mainly diffuse sources)	<i>0.5</i>
Used in the open environment	<i>1</i>

**Table 6:** Criterion used to calculate tonnage multiplier (characteristic parameter for each study area).

<b>Data reference area and</b>	<b>Tonnage multiplier</b>
Scotland	<i>1</i>
UK	<i>0.1</i>
Europe	<i>0.02</i>
World	<i>0.01</i>

### 3. Fugacity Perspective

The concept of fugacity (“tendency to flee”) can be potentially very useful in identifying the static and dynamic behaviour of toxic substances in the environment. Fugacity can provide a useful framework that may be used to compute the partitioning of chemicals among the phases of an ecosystem and helps to understand phenomena such as biodegradation or bioaccumulation. In order to apply fugacity models, the environment is depicted as a large box with six compartments, named as the Unit World (see Table 7). First we must built a scenario in which it is possible to observe the chemical distribution. This tool is capable of implementation (at various levels of complexity) and could form the basis for a procedure to assess the likely environmental behaviour of new chemical substances that have the potential for displaying adverse environmental effects.

**Table 7:** Volumes and densities of compartments [17]

Compartment	Volume ( $V_i$ )m <sup>3</sup>	Density Kg/m <sup>3</sup>
Air	$9 \cdot 10^9$ (1 km <sup>2</sup> area x 6km height)	1.19
Soil	$4.5 \times 10^4$ (30% area x 15 cm depth)	1500
Water	$7 \times 10^6$ (70% area x 10 m depth)	1000
Biota	7 (Water volume x 1 mg/L)	1000
Suspended sediment	35 (Water volume x 5 mg/L)	1500
Bottom sediment	$2.1 \times 10^4$ (70% area x 3 cm depth)	1500

The approach is also valuable in assisting the elucidation of the dominant processes responsible for a substance’s degradation or removal from the environment and in identifying the significant transfer process. Relative concentrations of a chemical in air, water and soil phases at equilibrium can be predicted from knowledge of the chemical’s partition coefficients (i.e. vapor pressure, Henry’s law constant and distribution coefficient). Each of the chemical’s partition coefficients describes a behaviour that may also be thought of in terms of chemical potential; when equilibrium partitioning among phases is attained, the chemical potentials in all phases are equal.

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The unknown fugacity in each compartment and the relevant concentrations can then be determined from the relationship:

$$C_i = Z_i \cdot f$$

- $C_i$  : chemical concentration in compartment i [ $\text{mol}/\text{m}^3$ ]
- $Z_i$  : fugacity capacity of compartment i [ $\text{mol}/\text{m}^3 \text{ Pa}$ ], (calculated according to the formulas listed in Table 8)
- $f$  : fugacity

**Table 8:** fugacity capacities of different compartments [17]

Environmental compartment	Z (fugacity capacity)
Atmosphere	$Z_a = 1/RT$
Water	$Z_w = 1/H$
Sorbed phases (soil, sediment and suspended solids)	$Z_s = K_p \rho_s / H$
Biotic phase	$Z_b = K_b \rho_b / H$

Where:

- R is the gas constant in  $\text{m}^3 \text{ Pa}/\text{mol } ^\circ\text{K}$  and T is the temperature ( $^\circ\text{K}$ )
- H is Henry's Law constant in  $\text{mol}/\text{m}^3 \text{ Pa}$ , Henry's Law constant is taken as  $P/s$  where P is saturation vapor pressure (Pa) and s is aqueous solubility  $\text{mol}/\text{m}^3$ .
- $K_p$  being the sorption coefficient in  $\text{m}^3$  of water/mole of sorbent, and  $\rho_s$  being the density of sorbent in  $\text{mol}/\text{m}^3$ .
- $K_b$  is the bioconcentration factor and  $\rho_b$  is the density of biota.

Chemicals move between phases by both diffusive and non-diffusive processes. The diffusive flux N ( $\text{mol}/\text{h}$ ) between two phases, 1 and 2, can be described by the equation:

$$N = D (f_1 - f_2)$$

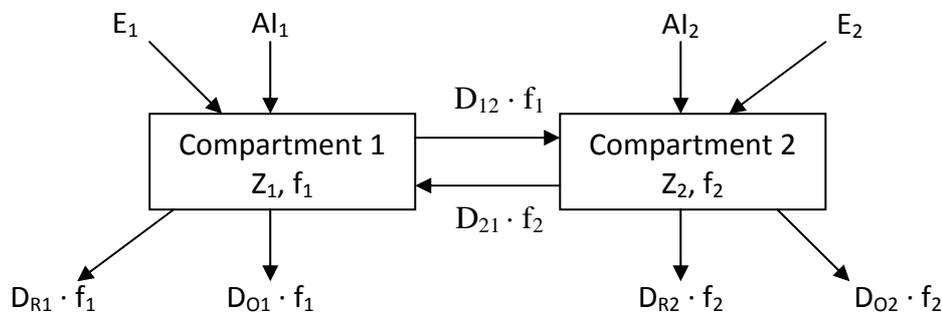
Where D is a transfer coefficient with units of  $\text{mol}/\text{h}\cdot\text{Pa}$  and  $f_1$  and  $f_2$  are the phase fugacities. The difference between  $f_1$  and  $f_2$  determines the direction of diffusive flux (but not non-diffusive flux) that takes place from high to low fugacity. D is a function of 2 values, interfacial areas, and diffusion properties in adjacent phases.

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When two adjacent phases are at equilibrium, their fugacities are equal ( $f_1 = f_2 = f_3 \dots f_i$ ) and partitioning can be described in terms of their Z values (a unique Z value exists for each chemical in each phase), as described in the equation:

$$C_1/C_2 = f \cdot Z_1 / f \cdot Z_2 = Z_1/Z_2$$

This equation allows to set relations between compartments for predicting pollutants concentrations within the different compartments and also how they migrate between them, how long they persist and how they are degraded. The procedure sets a mass balance (Figure 3):



**Figure 3:** Interactions between two compartment system

The respective mass balance equations are indicated below:

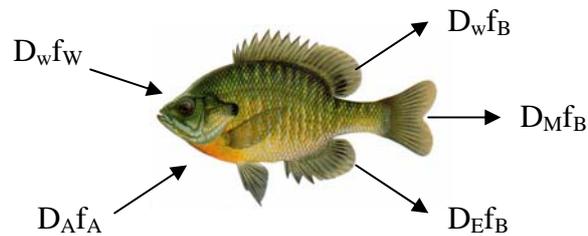
$$\frac{d(f_1 \cdot Z_1 \cdot V_1)}{dt} = E_1 + AI_1 + D_{21} \cdot f_2 + (D_{R1} + D_{O1} + D_{12}) \cdot f_1$$

$$\frac{d(f_2 \cdot Z_2 \cdot V_2)}{dt} = E_2 + AI_2 + D_{12} \cdot f_1 + (D_{R2} + D_{O2} + D_{21}) \cdot f_2$$

- $f_i$  fugacity in compartment  $i$  in Pa
- $Z_i$  fugacity capacity of compartment  $i$  ( $\text{mol}/\text{Pa} \cdot \text{m}^3$ )
- $V_i$  volume of compartment  $i$  ( $\text{m}^3$ )
- $t$  time (h)
- $E_i$  direct emission into compartment  $i$  ( $\text{mol}/\text{h}$ )
- $AI_i$  advective inflow into compartment  $i$  from outside the system ( $\text{mol}/\text{h}$ )
- $D_{ij}$  describes intercompartmental transport ( $\text{mol}/\text{Pa} \cdot \text{h}$ )
- $D_{Ri}$  describes degradation loss from compartment  $i$  ( $\text{mol}/\text{Pa} \cdot \text{h}$ )

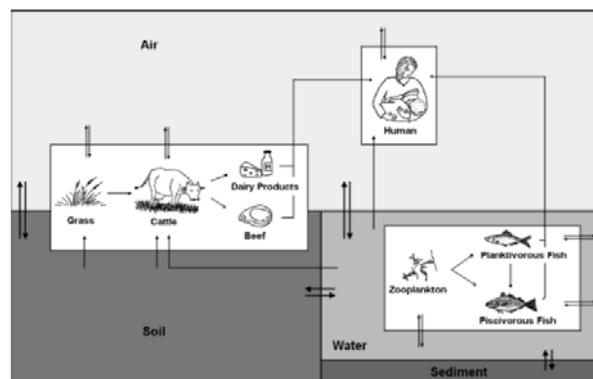
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- $D_{O_i}$  describes transport loss from compartment  $i$  (mol/Pa·h)



**Figure 4:** Contaminant uptake and clearance mechanisms (in terms of fugacities and  $D$  values, where:  $D_w$  is the respiratory exchange,  $D_A$  is net food uptake,  $D_M$  is the metabolism and  $D_E$  is the egestion) [18].

Fugacity models allow making more complex relationships between compartments. In Figure 4 just a unique organism has been taken into account, but if biomagnification occurs there is a potential for appreciable concentration increase at high trophic levels. Figure 5 shows a bioaccumulation model that describes chemical transfer through the aquatic and agricultural food chains to humans where each organism has its own interactions with the environment and also interactions through to the food chain, in which pollutants are transferred via predator-prey interactions.



**Figure 5.** Bioaccumulation model

#### **4. Conclusions**

This document represents the deliverable 3.2 of WP3 RISKCYCLE project and it is entitled "Overview of environmental factor influence over additive exposure and release into the environment".

Determining chemical exposure on the basis of environmental monitoring data would be the best and most reliable option. However, it would require widespread monitoring of all chemicals and unfortunately this is, in many cases, clearly unfeasible and economically unaffordable. Therefore, modelling has arisen as a promising alternative. During the last years different modelling approaches have been widely used allowing estimating the occurrence and adverse effects that chemicals may cause in both the environment and human health. However, prior to the implementation of any model, several influencing factors need to be known since they are often required as input parameters.

In the present document, the main factors affecting the chemical additives exposition, emission and fate have been compiled and discussed. For that purpose, they have been tentatively grouped into three classes, namely, intrinsic physical-chemical properties, environmental conditions and anthropogenic factors.

The integration of the three aforementioned factors has been illustrated using the fugacity concept developed by McKay as a representative example.

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