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ANALYSIS OF THE INFLUENCE OF SITE-SPECIFIC PARAMETERS IN THE CALCULATION OF CHARACTERIZATION FACTORS ASSOCIATED WITH CHEMICAL SUBSTANCES USING THE USETOX MODEL

Dissertação no âmbito do Mestrado em Engenharia Mecânica, na Área de Energia e Ambiente orientada pelo Professor Doutor José Manuel Baranda Moreira da Silva Ribeiro e Doutor Carlos Miguel Baptista Ferreira apresentada ao Departamento de Engenharia Mecânica da Universidade de Coimbra.

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Analysis of the influence of site-specific parameters in the calculation of characterization factors associated with chemical substances using the USEtox model

A dissertation submitted in partial fulfilment of the requirements for the degree of Master in Mechanical Engineering in the speciality of Energy and Environment

Análise da influência de parâmetros específicos locais no cálculo de fatores de caracterização associados a substâncias químicas utilizando o modelo USEtox

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Abstract

Environmental research related with emissions of various chemical substances often neglects the differences in the environmental characteristics of the emission site, analyzing the emission in an equal way, regardless of the region where it is released. It is important to take a further step and use this information to assess the environmental and toxicological impacts of this contamination, in a life-cycle perspective to avoid unexpected problems, taking into account these differences. The Life-Cycle Assessment (LCA) methodology can be employed to quantitatively assess the environmental impacts associated with chemical substances emissions. One issue that is necessary to consider when addressing the LCA methodology applied to substance emissions, is the site-specific parameters of the emission site. These can influence on a large scale the environmental burdens, mainly toxicological impacts, associated with the emission and, therefore, it is a topic needs to be addressed.

The USEtox model provides characterization factors for human toxicological and freshwater ecotoxicological impacts of chemical emissions in life cycle assessment. The aim of this thesis is to demonstrate the importance of assessing these characterization factors, taking into account the site-specific environmental parameters of the emission site, and understand the magnitude of the variation of the results between different regions. For that purpose, an evaluation and comparison of the characterization factors of substances emitted in different regions of the world is performed, in order to identify the cause of the potential variation between different regions. The USEtox model is used to assess the characterization factors of substances for the various regions: Europe; Northern Europe and Northern Canada; Central Asia; Southeast Asia; Oceania; Africa; USA and Southern Canada; Latin America; and the USEtox default region in which are analyzed the fate factors, intake factors and effect factors of chemical substances. Only the fate factors and intake factors presented variations, with different magnitudes, between the different regions, since these are dependent on the site-specific parameters of the emission site. Effect factors are only related to the toxicity of the substance under analysis. For the present study, five substances with different chemical characteristics were chosen: four organic substances, formaldehyde, allyl alcohol, octane and dioctyl terephthalate; and an inorganic substance, lead.

From the main results of this thesis, it was concluded that, in fact, site-specific parameters influence on a visible scale the results presented for the selected substances. These were obtained taking into account one emission for rural air and another for natural soil. Site-specific parameters such as rain rate, influence the persistence of substances in soil, this is, the fate factor in this compartment, reducing this value by increasing the degradation rate and promoting the transport of the substance to other compartments in which its persistence is lower. On the other hand, increases their persistence in aquatic compartments such as fresh water and sea water and contributes to the migration of substances to these compartments; the increase in the value of land area revealed to increase the persistence of substances in soil compartments; the human population has a huge influence on exposure to all substances, increasing the intake factor in all the exposure routes of inhalation and ingestion; the parameters associated with production based-intake rates such as the consumption of fish and agricultural products from above or below-ground production influence the amount consumed of a given substance and are, therefore, parameters that will lead to different results of intake factor, depending on the region of emission. The results also vary between different substances since their chemical characteristics determine the compartments where they will tend to be deposited and also their presence on the different routes of exposure. For example, considering an emission to rural air, lead persists more in soil compartments and is associated with ingestion routes such as above-ground production; the octane, due to its volatility, persists in air compartments so it will be present in inhalation exposure routes.

The conclusions drawn can aid in providing tailored and supported decisions in order to understand how site-specific parameters influence the substances characterization factors associated with emissions, released in different regions.

Keywords: Characterization factors of substances, chemical substances emissions, life-cycle assessment, site-specific parameters, toxicological impacts, USEtox model.

Resumo

A investigação ambiental relacionada com as emissões de várias substâncias químicas negligencia frequentemente as diferenças nas características ambientais do local de emissão, analisando as emissões de igual forma, independentemente da região de emissão. É importante dar mais um passo e utilizar estas informações para avaliar os impactes ambientais e toxicológicos desta contaminação, numa perspetiva de ciclo de vida para evitar problemas inesperados, tendo em conta estas diferenças. A metodologia de avaliação de ciclo de vida (ACV) pode ser utilizada para avaliar quantitativamente os impactes ambientais associados às emissões de substâncias químicas. Um tema que é necessário ter em consideração ao abordar a metodologia de ACV aplicada às emissões de substâncias, são os parâmetros específicos do local de emissão. Estes podem influenciar, em grande escala, os problemas ambientais, principalmente os impactes toxicológicos, associados à utilização de munições e, por conseguinte, é um tema que requer atenção cuidada.

O modelo USEtox fornece fatores de caracterização para os impactes toxicológicos humanos e ecotoxicológicos de água doce das emissões químicas na avaliação do ciclo de vida. O objetivo desta tese é demonstrar a importância de avaliar estes fatores de caracterização, tendo em conta os parâmetros ambientais específicos do local de emissão, e compreender a magnitude da variação dos resultados entre diferentes regiões. Para o efeito, realiza-se uma avaliação e comparação dos fatores de caracterização de substâncias emitidas em diferentes regiões do mundo, a fim de identificar a causa da variação potencial entre as diferentes regiões. O modelo USEtox é utilizado para avaliar os fatores de caracterização das substâncias para as diferentes regiões: Europa; Norte da Europa e Norte do Canadá; Ásia Central; Sudeste Asiático; Oceânia; África; EUA e Canadá do Sul; América Latina; e a região padrão do USEtox em que são analisados os fatores do destino, fatores de intake e fatores de efeito de substâncias químicas. Apenas os fatores de destino e os fatores de intake apresentaram variações, com diferentes magnitudes, entre as diferentes regiões, uma vez que estas dependem dos parâmetros específicos do local de emissão. Os fatores de efeito estão apenas relacionados com a toxicidade da substância em análise. Para este estudo, foram escolhidas cinco substâncias com características químicas diferentes: quatro substâncias orgânicas, formaldeído, álcool alílico, octano e tereftalato de dioctilo; e uma substância inorgânica, chumbo.

A partir dos principais resultados desta tese, concluiu-se que, de facto, os parâmetros específicos do local influenciam numa escala visível os resultados apresentados para as substâncias selecionadas. Estes foram obtidos tendo em conta uma emissão para o ar rural e outra para o solo natural. Parâmetros específicos do local, como a taxa de chuva, influenciam a persistência de substâncias no solo, isto é, o fator de destino neste compartimento, reduzindo este valor aumentando a taxa de degradação e promovendo o transporte da substância para outros compartimentos em que a persistência desta é menor. Por outro lado, aumenta a persistência em compartimentos aquáticos, como a água doce e a água do mar, e contribui para a migração de substâncias para estes compartimentos; o aumento do valor da superfície terrestre revelou aumentar a persistência de substâncias nos compartimentos do solo; a população humana tem uma enorme influência na exposição a todas as substâncias, aumentando o fator de intake nas diferentes rotas de exposição de inalação e ingestão; os parâmetros associados às taxas de ingestão baseadas na produção, tais como o consumo de peixe e produtos agrícolas de produção acima ou abaixo do solo, influenciam a quantidade consumida de uma determinada substância e são, por conseguinte, parâmetros que conduzirão a diferentes resultados do fator de intake, dependendo da região de emissão. Os resultados variam também entre diferentes substâncias uma vez que as suas características químicas, determinam os compartimentos onde estas terão tendência em se depositar e também a sua presença nas diferentes rotas de exposição. Por exemplo, considerando uma emissão para o ar rural, o chumbo persiste mais nos compartimentos de solo, estando associado a rotas de ingestão como a produção acima do solo; o octano, devido à sua volatilidade, persiste em compartimentos de ar, logo estará associado a uma rota de exposição de inalação.

As conclusões retiradas podem ajudar na concessão de decisões adaptadas e apoiadas, a fim de compreender como os parâmetros específicos do local influenciam os fatores de caracterização de substâncias associadas a emissões, libertadas em diferentes regiões.

Palavras-chave: Avaliação de ciclo de vida, emissões de substâncias químicas, fatores de caracterização de substâncias, impactes toxicológicos, modelo USEtox, parâmetros específicos locais.

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List of Symbols

h – Mixed height

V – Volume

A - Area

ρ – Bulk density

m - mass

Acronyms

abv.gr.prod.: Above ground production

agr.soilC: Agricultural soil at the continental scale

agr.soilG: Agricultural soil at the global scale

airC: Rural air at the continental scale

airG: Rural air at the global scale

airI: Indoor air at the indoor scale

airU: Urban air at the urban scale

Areafrac: Fraction of area

BAF: Bioaccumulation factor

blw.gr.prod: Below ground production

BTF: Biotransfer factor

canc: Cancerous

CFs: Characterization factors

CTUe: Comparative toxic unit for ecosystems

CTUh: Comparative toxic unit for human health

DALY: Disability Adjusted Life Years

dr.water: Drinking water

EC_{50}: Half maximum effective concentration

eco: Ecosystem

ED_{50}: Median effective dose

EF: Effect Factor

FF: Fate Factor

fr: Fraction

fr.waterC: Freshwater at the continental scale

fr.waterG: Freshwater at the global scale

iF: Intake Factor

ing: Ingestion

inh: Inhalation

IR: Intake Rate

k_{degA}: Rate constant degradation in air

k_{degSd}: Rate constant degradation in sediment

k_{degSl}: Rate constant degradation in soil

k_{degW}: Rate constant degradation in water

K_{dissP}: Rate constant dissipation in above-ground plant tissues

K_{DOC}: Dissolved organic carbon-water partition coefficient

K_{H25C}: Henry’s law coefficient (at 25°C)

K_{OC}: Organic carbon-water partition coefficient

K_{OW}: Octanol-water partition coefficient

Kp_{sd}: Partitioning coefficient between sediment particles and water

Kp_{Sl}: Partitioning coefficient between soil particles and water

Kp_{ss}: Partitioning coefficient between suspended solids and water

LCA: Life-Cycle Assessment methodology

LCI: Life-Cycle Inventory

LCIA: Life-Cycle Impact Assessment

MW: Molar mass

nat.soilC: Natural soil at the continental scale

nat.soilG: Natural soil at the global scale

noncanc: Non-cancerous

oceanG: Ocean at the global scale

P: Population head count

PAF: Potentially Affected Fraction of species

PDF: Potentially Disappeared Fraction of species

P_{vap25}: Vapour pressure (at 25ºC)

seawaterC: Coastal sea water at the continental scale

Sol_{25}: Water solubility (at 25ºC)

Temp: Temperature

XF: Exposure Factor

xp: Exposure pathway

1. INTRODUCTION

The main motivation of this thesis is the evaluation and comparison of characterization factors of substances associated with emissions released by the use of energetic materials (e.g. ammunition) in regions with different environmental characteristics. Although the evaluation is made at the level of the characterization factors with a wider range of substances beyond those emitted from the use of energetic materials, these influence the potential toxicological impacts, so the contextualization about this topic is addressed.

The possible environmental consequences associated with emissions of chemical substances, can arise in any of the life cycle phases of products (i.e. production phase, use phase and end-of-life phase) or in other activities (e.g. military activities). An assessment carried out for a small calibre ammunition, showed that the production phase has a higher contribution to the environmental impact categories, whilst use phase shows a higher contribution to the toxicological impact categories. The impacts associated with the production phase are essentially determined by the amount of resources used (raw materials and energy). For the Human Toxicity categories, the impacts are essentially associated with the emissions from firing (use phase) (Ferreira et al., 2016).

The impacts associated with the direct burdens related to the gaseous or particle emissions originated from the ammunition firing and/or detonation (Ferreira et al., 2017), are mainly associated with the presence of toxic substances (e.g. lead). For instance, emissions of metals (such as lead, copper and nickel) during the use of small calibre ammunitions in military training and hunting have been identified as a major problem from an environmental and toxicological point of view (Ackermann et al., 2009; Tsuji et al., 2008). In fact, small calibre shooting ranges can contain concentrations of lead, that can be poisoning to birds due to unintentional consumption of lead particles or animals that are contaminated with fragments of lead bullets (Fisher et al., 2006; Green & Pain, 2012; Helander et al., 2009). The poisoning of wild game birds with lead and other heavy metals also presents a potential risk for human health due to consumption of meat contaminated (Green & Pain, 2012). More-over, the direct inhalation of heavy metals and combustion residues by shooters is also a reason for serious concern (Bonanno et al., 2002).

The emissions generated through the life cycle of a product occur in many places, within multiple media (air, water, soil) and cause impacts on local environmental parameters

(Owens, 1997; Reap et al., 2003). Unlike global impacts, such as ozone layer depletion and global warming, those affecting local, regional, and continental scales require spatial information to accurately associate sources with environments of varying parameters with different sensitivity. However, most assessments continue to ignore spatial considerations, despite a decade of developing methods designed to fix these problems (ISO 14040:2006; Potting & Hauschild, 2006). This topic constitutes an important limitation in the study of the LCIA and it will be addressed in detail.

In this thesis, the focus will be on the use phase, that is, the moment when the emission of a substance is released to the environment. For example, at the time of firing, the substances are released into different media such as water, air or soil, and depending on the site-specific environmental parameters, it may, or may not, disperse to other media. Still on the fate of the substances after the shooting, these tend to volatilize or to be more persistent in the soil or water, depending on their physical and chemical characteristics. In this work, the main focus is to analyze the variation of environmental and human characterization factors associated with chemical substance emissions in different locations of the world and to conclude about the causes of the variation of these factors. This will require the use of an impact model that considers the substance emission compartment, the location (on an urban, global or continental scale) and the possibility of dispersion to other compartments. Respecting these conditions and others that will be described in detail in subchapter 3.1, the USEtox model was used.

Briefly, the USEtox model, assess the toxicological effects of a chemical emitted into the environment by analysing a cause–effect chain that links emissions to impacts through three steps: environmental fate, exposure and effects. The links of this cause-effect chain are modelled using matrices populated with the corresponding factor for the three steps mentioned (Rosenbaum et al., 2008). The fate model links the quantity released into the environment to the chemical masses (or concentrations) in a given compartment (Fantke et al., 2017). Human exposure factors reflect the rate at which a pollutant is able to transfer from a receiving compartment into the human population through a series of exposure pathways (Fantke et al., 2015). Human effect factors in USEtox relate the quantity taken in by the population via ingestion and inhalation to the probability of adverse effects (or potential risk) of the chemical in humans (Rosenbaum et al., 2008). The multiplication of these three factors results in a substance-specific characterization factor (CF), that combine exposure potential and toxicity to represent the relative contribution of the substance to health and ecosystem impacts (Hauschild et al., 2008).

This method still has inherent limitations, the main being the fact that the LCA methodology does not address site-specific impacts. Traditional LCA studies use average data from specific regions to calculate the environmental impacts with global effects (e.g. climate change, abiotic depletion) (ILCD Handbook; Sala et al., 2011). Since the toxicological impacts are strongly influenced by site-specific parameters, it is a challenge to evaluate those impacts in LCA studies (Ferreira et al., 2019b).

The methodology for the use of life cycle assessment (LCA) on specific locations can be an appropriate tool to overcome these limitations by quantifying the environmental consequences associated with contamination of this space in a great resolution. With LCA studies the impacts can be quantified and also identified what is contributing to them; thus, it allows the entities responsible for facilities to know the impacts in order to reduce or mitigate them. In addition, LCA studies can be applied to predict impacts (e.g. to assess the potential impacts of using military artillery in shooting ranges to prevent future contamination) (Ferreira et al., 2019).

1.1. Scope and objectives

The main objective of this thesis is to address the potential influence of the site-specific parameters of different regions to the calculation and assessment of characterization factors associated with chemical substances emissions. In this work will be used 5 different substances whose emission is considered in 9 different regions (including the USEtox default region), directly to the rural air and natural soil compartments.

For that purpose, is performed an evaluation and comparison of the characterization factors associated with the emissions of chemical substances in different regions of the world, in order to identify the cause of the potential variations of results (e.g. type of soil; different eating habits; type of chemical released). In order to understand if the model is sensible to the site-specific conditions, new USEtox model regions will be developed and described in detail. After that, they will be used to perform a sensitivity analysis to the different parameters that can influence the characterization factors. From this analysis it is possible to conclude how the characterization factors of substances vary with the variation of the site-specific parameters, specifically the fate factor and the intake factor.

1.2. Thesis organization

The methodology used consists of a bibliographic analysis to understand the topics addressed: initially, the LCA methodology, as well as its limitations and its applicability for for the assessment of toxicological impacts on specific regions, is addressed; posteriorly, the USEtox model is presented to understand its framework on the calculation of substance characterization factors, based on the physicochemical properties of the substances and the site-specific parameters of regions. The model is used to calculate and compare the characterization factors associated with chemical substances in different areas of the world using various types of chemicals. Thus, the USEtox section of landscape data is aborded in detail, including the justification for the choice of regions and the explanation about how each site-specific parameter used for the definition of these regions is obtained (and their limitations). The study substances are also selected for comparison. In addition, the definition of specific regions, varying the site-specific parameters of USEtox default region and a sensitivity analysis to those parameters is performed, to understand how CFs vary with the variation of local environmental characteristics. Finally, the results obtained are analyzed in order to present improvement solutions and draw some conclusions.

This thesis is divided into five chapters and is structured as follows:

Chapter 1 presents the theoretical framework, the subject and the purpose of the development of the thesis. It is also presented a justification for the choice and remarks about the importance of the subject, and the objectives outlined for the work to be developed. Finally, a description of the methodology followed for the development of the work and, briefly, its structure is also carried out.

Chapter 2 reviews the literature on the life cycle assessment methodology and present the USEtox model, the method used to calculate the characterization factors associated with substance emissions. Firstly, is presented a review addressing the life-cycle assessment methodology in general, based on its definition according to ISO standards. The research gaps of the application of the LCA methodology for assessing the toxicological impacts on specific regions are also presented. Later in this chapter is described the motivation and the needs for the creation of the USEtox model, as well as its general framework.

Chapter 3 presents the USEtox model framework in detail, the explanation for the calculation of characterization factors, including the fate factors, exposure factors and effect factors. It also describes the site-specific parameters section of USEtox. Firstly, a description of the world regions in the USEtox and the site-specific parameters used for the selected regions are presented. This part includes: a description of the IMPACT World model, used for the definition and characterization of the regions present in the USEtox; the selection of regions for evaluation; a detailed description about the obtaining method of each of the site-specific parameters characterizing the regions, as well as the associated limitations and simplifications. Later, in this chapter, is explained the procedure followed in the sensitivity analysis to site-specific parameters, whose results are presented and discussed in chapter 4. At the end of this chapter is selected the substances to be analyzed and a brief description about the type of chemical they represent.

Chapter 4 consists in the presentation and discussion of the results obtained from the practical research of this thesis, using the USEtox model. Includes the results of fate factors, intake factors and effect factors for all selected regions. It also includes the results of the sensitivity analysis to the variation of site-specific parameters and comparison of the results of the selected regions with the default region of USEtox.

Chapter 5 summarises the main findings related to the objectives of this thesis and provides recommendations for future research.

2. STATE-OF-THE-ART

2.1. Life-cycle assessment methodology

Life-cycle assessment (LCA) methodology follows the life-cycle principle in which the potential environmental and toxicological impacts of a product (or system) is quantitatively assessed throughout its life-cycle. This means that LCA studies encompass all the life-cycle phases, including the design, procurement, manufacturing, usage, disposal and transport between the different phases (ISO 14040:2006) – Figure 2.1.

Figure 2.1. Life-cycle assessment methodology.

Life-cycle assessment methodology, as described in the ISO standards, has four interconnected phases (Figure 2.2): the goal and scope where the main objective and purpose of the study is defined, including the identification of the product system boundaries and a functional unit, this is a reference that relates the system inputs and outputs and it is required to ensure comparability of results between different LCA studies; the inventory analysis (LCI) in which the inputs and outputs necessary to meet the goals of the study are collected and compiled, in this step is given a description of material and energy flows within the product system and especially its interaction with environment, consumed raw materials, and emissions to the environment; the life-cycle impact assessment that converts the inventory data into environmental impact values according to various methods, the importance of every impact category is assessed by normalization and eventually also by weighting; and the interpretation where the results are discussed and conclusions are drawn providing recommendations to decision makers. This latter step involves critical review, determination of data sensitivity, and result presentation (Muralikrishna & Manickam, 2017).

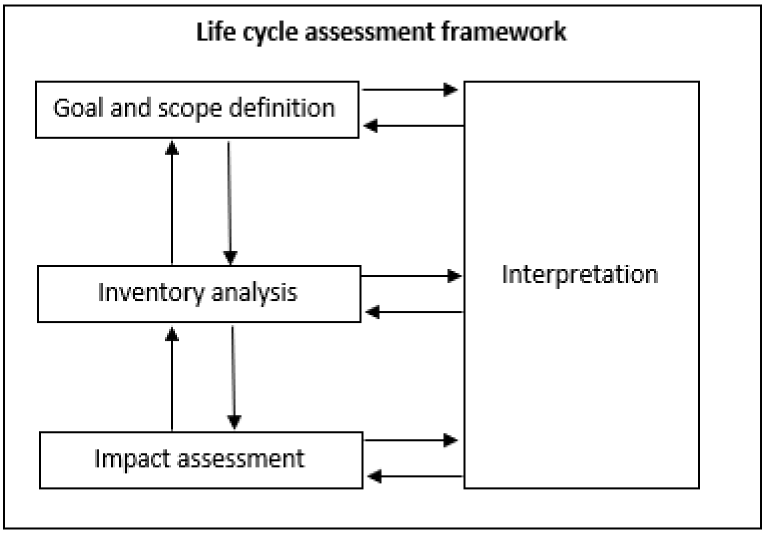

Figure 2.2. Stages of an LCA according to the ISO 14040:2006.

The major advantage of performing a LCA study is the opportunity to assess quantitatively the environmental and toxicological impacts of products or activities and identify the contributors to those impacts. With this information, opportunities to improve the environmental performance of products are identified, which life-cycle phase presents a higher contribution to the impacts are determined; and different products or technologies with the same function can be compared (Ferreira et al., 2019).

In the particular case of shooting ranges, the use of LCA will allow shooting range managers knowing the main environmental impacts associated with the use of ammunition as well as defining strategies to manage or mitigate those burdens (Ferreira et al., 2017).

The focus of this thesis is in the calculation and assessment of characterization factors associated with chemical substances (LCIA phase), mainly the exploitation of a LCIA model used for the assessment and calculation of these factors resulting from emissions to the regions defined with different site-specific parameters. At this phase of the LCA a process is defined to characterise and assess the effects of the environmental interventions identified in the life-cycle inventory (Heijungs & Hofstetter, 1996). USEtox is the main example of a life-cycle impact assessment model that can provide the information required to assess the characterization factors associated with substance emissions (Ferreira et al., 2019b), which is described in more detail in subchapter 3.1. This model use characterization factors to evaluate and quantify the toxicological impacts.

USEtox calculates a characterization factor for human toxicity as cumulative cases of either cancer or non-cancer health outcomes per kg of contaminant emission (cases per kg emitted), and a characterization factor for freshwater aquatic ecotoxicity impacts as the potentially affected fraction (PAF) of aquatic species integrated over the exposed water volume (m^3) and time (d), PAF·m^3·d per kg emitted (Fantke et al., 2017). Ultimately, the human health and ecotoxicity outcomes are described using a Comparative Toxic Unit (CTU) approach, to justify the comparative nature of the characterization factors. The characterization factors are assessed by three calculation steps. These sequentially provide a fate factor (FF), quantifying how the contaminant is dispersed in the environment, an exposure factor (XF), quantifying human and/or ecological system exposition with environmental media, and an effect factor (EF), quantifying the potential effects for humans or aquatic species (Fantke et al., 2015; Rosenbaum et al., 2008).

The resulting characterization factor (CF) that is required for the impact score for either human health or ecological impacts is generally defined as the combination of these three factors:

$$\boldsymbol{CF = FF \times XF \times EF} \tag{2.1}$$

This formula covers two major aspects, related to the environmental fate and behaviour of chemicals (FF and XF), and related to human or ecological effects (EF).

2.2. Limitations of the life-cycle assessment for assessing the toxicological impacts on specific regions

One of the limitations of the LCA methodology is that usually not addresses site-specific impacts. Traditional LCA studies use average data from specific regions to calculate the environmental impacts with global effects (e.g. climate change, abiotic depletion) (ILCD Handbook; Sala et al., 2011). Since the toxicological impacts are strongly influenced by site-specific parameters, it is a challenge to evaluate those impacts in LCA studies (Ferreira et al., 2019b).

The complexity of assessing toxicological and ecotoxicological characterization factors of substances (that links chemical emissions to impacts on humans and/or freshwater ecosystems) is due to the dependence on emission patterns, chemical properties, geographical characteristics and various other parameters (Hollander et al., 2009; Sala et al., 2011). The LCA studies that included site-specific information concluded that the conventional models (non-spatial) underestimate or overestimate the toxicological impacts by some orders of magnitude for some chemicals (Gandhi et al., 2011; Pennington et al., 2005; Sala et al., 2011). Consequently, the inclusion of higher spatial resolution could potentially reduce uncertainty in the calculation of toxicological impacts (Manneh et al., 2010).

Site-specific parameters have a strong influence on the variation of characterization factors of substances and toxicological impacts, as they influence the behaviour of chemicals when released into the environment. This is the reason why it is important to define an impact model that addresses local environmental parameters. Atmospheric, topography and hydrology variations are capable of influencing life cycle assessments studies and compromise its conclusions. Region specific impact score formulations for airborne deposition of eutrophying compounds contain factors for runoff, a factor strongly influenced by topography (Huijbregts & Seppälä, 2000). Estimations of water quantity impacts (e.g., drought stress on biomass, well failure, etc.) depend upon spatially explicit hydrology models or data sets (Heuvelmans et al., 2005; Reap et al., 2004). Groundwater contamination from landfills has been found to vary by as much as four orders of magnitude based on geological conditions and geographic location (Hellweg, 2001).

2.3. USEtox model presentation

The need for developing toxicity-related characterization factors has been addressed over the last 20 years by deriving several characterization models, which vary in their scope, applied modelling principles, units and magnitudes (Hauschild et al., 2008). These characterization models cover a limited number of substances. Before the development of USEtox model, a LCA practitioner to assess chemical-related impacts in the impact assessment was hindered by substances in the LCI phase for which no characterization factor was available from any of the previous models. Also, several models may have published characterization factors but often with substantial variations between them (Fantke et al., 2017). This undesirable situation was the motivation on which a Task Force on Toxic Impacts under the UNEP-SETAC Life Cycle Initiative launched a comparison and accordance of existing characterization models in order to:

1. Identify which differences in the old characterization models cause the observed differences in their characterization factors;
2. Develop a scientific consensus about good modelling practice based on the identified influential differences;
3. Harmonize the old characterization models removing unintended but influential differences; and
4. Develop a scientific consensus model based on the findings from the comparison of the old characterization models (Rosenbaum et al., 2008).

The new model should follow these new characteristics:

a. Being parsimonious (as simple as possible, as complex as needed) containing only the model elements which were identified as the most influential in the comparison of the existing characterization models;

b. Being transparent and well documented, including the reasoning for model choices;

c. Falling within the range of existing characterization models;

d. Being endorsed by the developers, providing a tailored and supported decisions through evaluation against a broad set of existing models (Hauschild et al., 2008).

The result of the scientific consensus model development is the USEtox model and its associated set of characterization factors. Continued conceptual and technical developments, as well as increased availability of data has resulted in the current update of USEtox 2.12.

The USEtox model is an environmental impact model based on a scientific consensus to characterize human and ecotoxicological impacts of chemicals in life cycle impact assessment (Fantke et al., 2017). The goal of developing this impact model was to improve the assessment and management of chemicals in the global environment. This was achieved by further developing, evaluating, applying and discriminating the USEtox model, which describes the environmental fate, exposure and effect parameters for human toxicity and ecotoxicity of chemicals (Westh et al., 2015), as shown in Figure 2.3.

The result is an Excel sheet with data from recommended and interim characterization factors. With them it is possible to identify which are the substances with priority importance and the mechanisms of transfer between other compartments. The current version of USEtox contains a broad coverage of assessment situations through a wide array of required input data and model extensions (Fantke et al., 2017).

Focusing on the impact categories “human toxicity” and “ecotoxicity”, emission inventories for the life cycle of a product often results in the need to consider the potential impacts of hundreds or thousands of substances, most of them frequently used in the life cycle of products on the market (Judson et al., 2009; Wambaugh et al., 2013). Many of these substances have the potential to damage humans or ecosystems when released to the environment. There is thus the need to derive and use characterization factors for the human toxicity and ecotoxicity impact categories for all potentially relevant chemicals (Fantke et al., 2017).

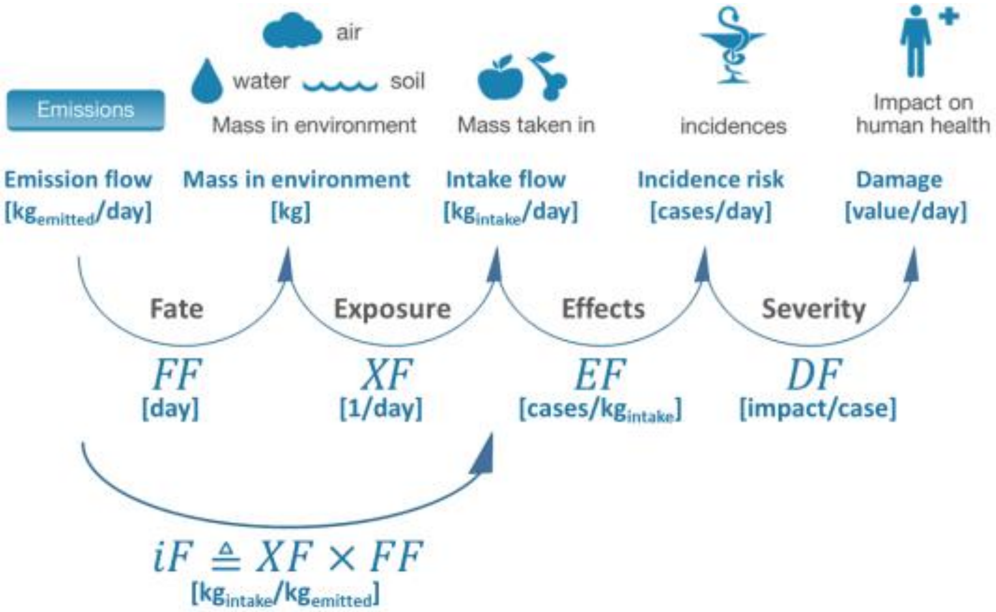

Figure 2.3. Framework for characterizing toxicity impacts with USEtox. Source: (Fantke et al., 2017).

3. MATERIALS AND METHODS

In this chapter, the USEtox model, which is the method used to assess the characterization factors associated with the emission of chemical substances, is explained in detail. Firstly, the framework for calculating the substance characterization factors is presented, followed by the explanation of each of the calculated factors.

The transfer of substances between compartments in USEtox is defined on a continental scale, global scale and urban scale, as represented in Figure 3.2. In subchapter 3.2 and 3.3 it is described in detail how each of the site-specific parameters incorporated in USEtox is obtained, the databases used, and the definitions involved, as well as the limitations associated with the use of this data. A sensitivity analysis to site-specific parameters will also be performed, through the creation of artificial regions, in order to understand how the characterization factors of the substances vary with the variation of these parameters.

To contextualize about the site-specific parameters described for the regions defined in USEtox, information on these parameters is presented in Annex A. Respectively, in Table A1, the regions described in the USEtox model and from Table A2 to Table A6 are presented all the defined site-specific parameters, respectively for all the present scales: continental scale, global scale, urban scale, human exposure and for production-based intake rates.

To define and parametrize the regions implemented in USEtox, where the differences in the site-specific parameters can be observed inter-regionally, this model uses a tool that includes the fate of the pollutant in multiple environments, cover multiple routes of exposure, and account for areas of high intensity exposure and cross-border transport. This solution was then developed under the name IMPACT World, whose concept is explained in detail in subchapter 3.2.1. The USEtox model defines a total of 17 subcontinental regions and 8 grouped continental regions, from these 9 were selected, including the USEtox default region, and their presentation is made in subchapter 3.2.2. Since the USEtox describes a vast number of regions, its selection was mainly made in order to cover a wide variety of areas of the world but selecting a small number of regions.

Now introducing the site-specific parameters of each region, these are several, thus attributing unique characteristics to each region. Most parameters are variable between regions, but some of them, due to limitations or simplifications of the model, are assumed to be the same in all regions and have a value equal to that defined for an USEtox default region (e.g. temperature, soil erosion). To calculate various site-specific parameters, it was necessary to use space information programs such as GIS and tropospheric chemistry models that provide wind speed averages like GEOS-Chem. Besides this, databases such as FAO and FAO FishSTAT, were used to obtain parameters related to production-based intake rates. All information on the obtaining of the site-specific parameters defined in USEtox is presented in subchapter 3.2.3.

Later, it is explained how sensitivity analysis to site-specific parameters will be performed, varying them and understanding how changing these values in small and large magnitudes influences the behaviour of substances when released into the environment. At the end of this chapter is selected the substances to be analyzed and a brief description about the type of chemical they represent.

3.1. USEtox model description

3.1.1. Calculation of characterization factors in USEtox model

Assessing the human toxicological or ecotoxicological effects of a chemical emitted into the environment implies the analysis of a cause-effect chain that links chemical emissions to impacts on humans and/or freshwater ecosystems through three assessment steps: environmental fate, exposure, and human toxicological and freshwater ecotoxicological effects (Fantke et al., 2017). The framework applied in the USEtox model for the calculation of each factor in presented in Figure 3.1 . Each one of these factors will be explained in detail in the following subchapters.

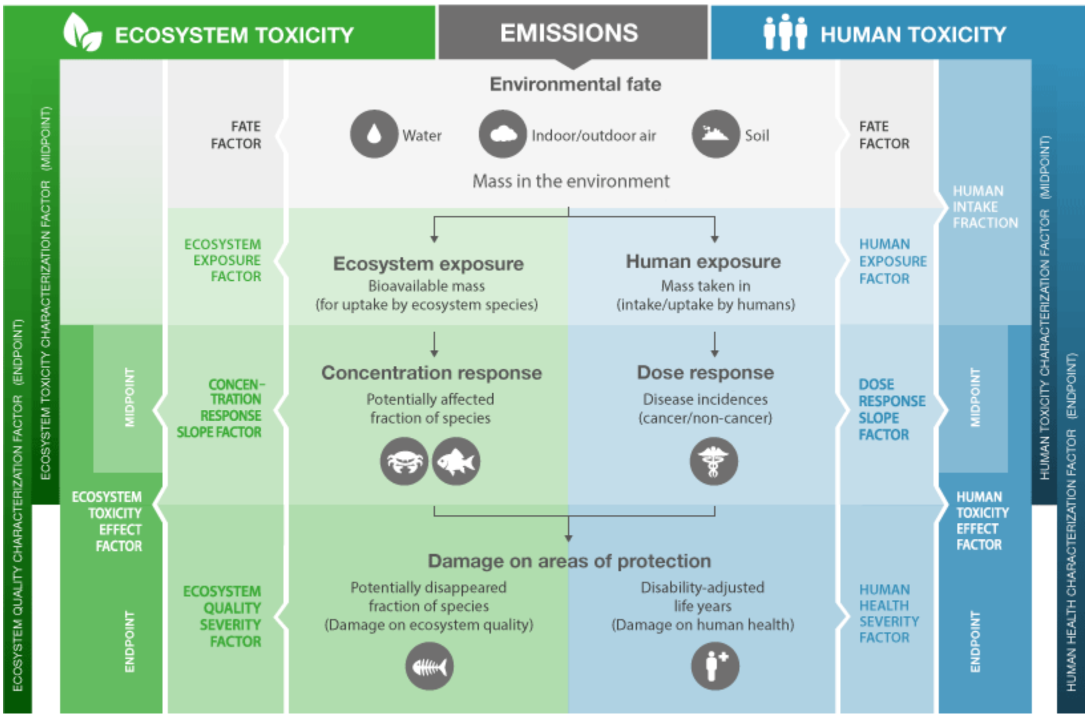

Figure 3.1. Framework for characterizing human toxicity and freshwater toxicity impacts in USEtox. Source: (Fantke et al., 2015).

An emission compartment-specific toxicity impact score is calculated by multiplying the mass of a substance emitted in a given compartment with the corresponding toxicity midpoint or endpoint characterization factor (Fantke et al., 2015).

The characterization factors must be used in a way that reflects the large variation, often various orders of magnitude, between substance characterization factors (Rosenbaum et al., 2008). In practice, this means that for practitioners, the life-cycle toxicity scores enable the identification of all substances that have the greatest contribution to the total score, and identify the others whose impacts are not significant for the considered application. Once these most important substances have been identified further analysis can be carried out on the components responsible for those emissions (Fantke et al., 2015). Due to its simple and transparent matrix-based calculation framework, USEtox will also allow identification of the main exposure pathways, (e.g. inhalation, drinking water ingestion, ingestion of various food items including direct residues of pesticides in agricultural crops) as well as the relative importance of potential carcinogenic and non-carcinogenic effects in the overall score (carcinogenic and non-carcinogenic aggregated assuming equal weighting at midpoint level or impact-specific weighting at endpoint level, where in the latter carcinogenic and non-carcinogenic impacts are weighted differently) by analysing the resulting characterization factors for a selected substance (Fantke et al., 2015).

3.1.1.1. Distinction between recommended and interim characterization factors

The provided characterization factors can be classified as “recommended” or “interim”. Recommended factors are given for substances where the USEtox model is considered fully appropriate and the underlying substance data are of sufficient quality to support a recommendation based on scientific consensus (Hauschild et al., 2008). In cases where relatively high uncertainty in addressing fate, exposure and/or effects of a substance is expected, the related characterization factors are labeled as “interim”. In practice, this recommendation is given in cases where the substance is a metal, an organometallic chemical, an amphiphilic chemical (e.g. detergents) or when information on dissociation under environmental conditions could not be determined (Fantke et al., 2015). Also, for freshwater aquatic ecotoxicological characterization factors, these are recommended to be specified as «interim», if effect factors are based on species toxicity data covering less than three different trophic levels (positions of organisms on food chain) (Fantke et al., 2015). This is to ensure a minimum variability of biological responses and a greater reliability in the model. For human toxicological effects, is recommended that characterization factors be specified as “interim”, if effect factors are based on sub-acute data.

Interim CFs might be used in LCA studies, but with great caution and under the consciousness of their large inherent uncertainty. In the case that an LCA result is dominated by impact scores based on interim CFs, great caution is needed to proceed to their interpretation enhancing that these factors are neither recommended nor endorsed (Rosenbaum et al., 2008). Some characterization models ignore interim factors, however USEtox states: “Excluding interim characterization factors is in principle only meaningful on sensitivity analysis in life cycle assessment study”.

3.1.2. Fate

Regarding fate and behaviour, multimedia fate models are applied to determine contaminant environmental fate factors (FF). In this system, the impacted region is represented by a number of homogeneous compartments, each representing a specific part of the environment (i.e. atmosphere, water, soil) (Fantke et al., 2017).

The fate factor of a contaminant in a certain compartment is calculated by solving a set of mass balance equations that describe processes such as degradation and inter-compartment transfer. The fate factor represents the persistence of a chemical in the environment (expressed in days) as well as the relative distribution. For different chemicals, different processes are important in defining both fate and exposure. Which processes are the most important for a certain contaminant, depends on the physical-chemical properties of the corresponding substance. Also, the environmental conditions (e.g. temperature, precipitation intensity, etc.) influence both fate and exposure (Fantke et al., 2017).

In USEtox, different nested scales are specified:

- The indoor environment scale for household settings;
- The urban scale with the urban air compartment;
- The continental scale with the following compartments: air, freshwater, coastal sea, natural soil and agricultural soil;
- The global scale with the following compartments, air, freshwater, ocean water, natural soil and agricultural soil.

In Figure 3.2 a representation of the compartments in USEtox is presented, in which the indoor environment scale and urban scale are nested in the continental scale and the continental scale is nested in the global scale.

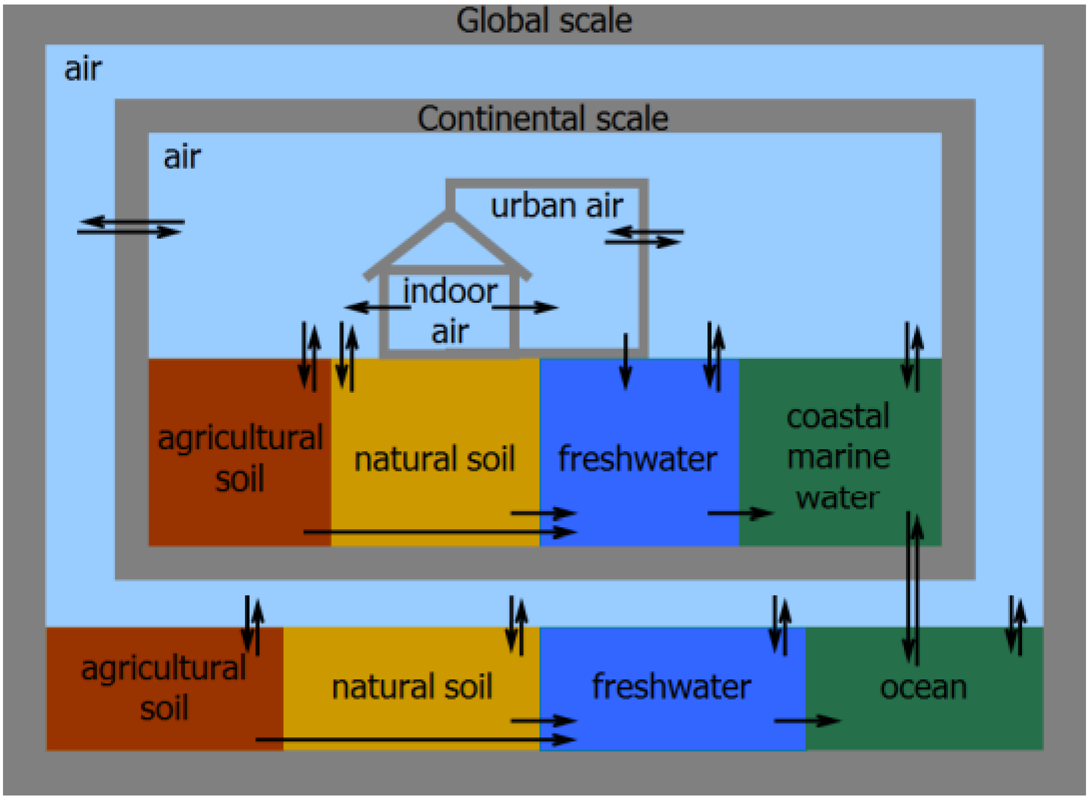

Figure 3.2. Representation of the USEtox nested compartments and their transfer processes. Source: (Fantke et al., 2017).

As USEtox encompasses the definition of different compartments, each one of them have different dynamics related to persistence of substances when released in one specific compartment as well as the transfer processes between them.

Air is treated in USEtox as a homogeneous compartment, consisting of a gas phase, an aerosol phase and a rainwater phase. The air in the system is not stagnant; it is continuously being transferred between different compartments. As the chemical is carried with these airstreams, this leads to "import" and "export" mass flows of the chemical to and from the system (Fantke et al., 2017).

The volume of the air compartment in the urban, continental and global scales, represented with the index “S”, may be obtained from:

$$V_{\mathrm{air[S]}} = A_{\mathrm{[S]}} \cdot h_{\mathrm{air[S]}} \tag{3.1}$$

with

$V_{air[S]}$: volume of the urban, continental and global air [m^3]
$A_{[S]}$: urban, continental and global system area [m^2]
$h_{air[S]}$: mixed height of the urban, continental and global air [m]

The mixing height is defined as the height above the surface along which a pollutant can be dispersed.

At the urban scale no water compartments are present, while at the continental and global scale there are two water compartments: a fresh water and a sea water compartment. In USEtox the water compartments are treated as homogeneous boxes, consisting of a suspended matter phase, a dissolved (colloidal) organic carbon (DOC) phase and a biota phase. The presence of suspended matter, DOC and biota influences the fate of chemicals in a very similar way to that of rainwater in the atmosphere. These phases attach the chemical, thus inhibiting it from taking part in mass transfer and degradation processes that occur in the water phase. Suspended matter behave as a physical carrier of the chemical across the sediment-water interface. Concentration ratios among suspended matter, DOC, biota and water are often close to equilibrium. For multimedia fate modelling, the water compartment is treated the same way as the air, sediment and soil compartments: that is at all times equilibrium is assumed among water, suspended matter, DOC and biota. The water compartments at the continental and global scales are continuously transferred with water (and biota, suspended matter and DOC) from outside that scale (Fantke et al., 2017)

The volume of the fresh and sea water compartments may be obtained from:

$$V_{w[S]} = A_{[S]} \cdot fr\_A_{w[S]} \cdot h_{w[S]} \tag{3.2}$$

with

$V_{w[S]}$: volume of continental and global fresh and sea water [m^3];
$A_{[S]}$: continental and global system area [m^2];

$fr\_A_{w[S]}$: area fraction continental and global fresh and sea water [-];
$h_{w[S]}$: mixed depth of continental and global fresh and sea water [m].

Ocean mixed layer depth is one of the most important quantities of the upper ocean because it defines the surface region with homogeneous characteristics of density that directly interacts with the atmosphere (Kara, 2003).

USEtox does not explicitly calculate concentrations in sediments. It does account for transport of substance between water and sediment via direct processes of adsorption/desorption and by sedimentation/resuspension of suspended particulate matter (Margni et al., 2004). The sediment phase is treated as a homogeneous phase, consisting of a water and a solid sub-phase. Equilibrium is assumed between the pore water and solid sub-phases of the sediment phase. The top layer of the sediment is considered to be well-mixed. If the sedimentation of particles from the water column is greater than the resuspension (net sedimentation), this top layer is continuously being refreshed. The older sediment layer, and the chemicals that are associated with the sediment with it, gets buried under the freshly deposited material (Fantke et al., 2017).

The volume of continental and global fresh and sea water sediment may be obtained from:

$$V_{\mathrm{wsd}[\mathrm{S}]} = A_{[\mathrm{S}]} \cdot fr\_A_{\mathrm{w}[\mathrm{S}]} \cdot h_{\mathrm{wsd}[\mathrm{S}]} \qquad (3.3)$$

with

$V_{wsd[S]}$: volume of continental and global fresh and sea water sediment [m^3];
$A_{[S]}$: continental and global system area [m^2];
$fr\_A_{w[S]}$: area fraction continental and global fresh and sea water [-];
$h_{wsd[S]}$: mixed depth continental and global fresh and sea water sediment [m].

Soil is the most stationary media and, as a result, the most spatially inhomogeneous of all environmental compartments. As described in earnest (https://www.earnest.ag/different-types-of-soil-different-uses/), there are many different soil types and differences in soil use, for example: silty soil is an excellent fertile ground for a large number of vines, grasses and flowers, due to great water draining properties; clay soil, usually drains poorly, meaning water will take a long time to filter through it. So it is, in general, an unsuitable soil to garden; etc. The fate of chemicals is determined largely by the characteristics that vary with the location (porosity, water content, organic matter content) which difficult the modelling. Also, soil usage is also a key factor determining whether the soil compartment can be contaminated directly with a chemical. One soil compartment may not be sufficient to reflect the role of "soil" in the multimedia fate of chemicals. USEtox, therefore, defines two separate soil compartments at the continental and global scale. One soil compartment is considered as "natural soil" and the other soil compartment as "agricultural soil", to differentiate the potential usages of the soil. At the urban scale, the area fraction of paved and non-paved surface is considered instead of soil compartment. Chemical flow from the soil to the air is dependent of the penetration depth of the chemical into the soil. Soil is treated as a homogeneous compartment, consisting of a gas phase, a water phase and a solid phase. The different soil phases are assumed to be in equilibrium at all times (Fantke et al., 2017).

The volumes of the soil compartments may be obtained from:

$$V_{\mathrm{sl[S]}} = A_{\mathrm{[S]}} \cdot fr\_A_{\mathrm{sl[S]}} \cdot h_{\mathrm{sl[S]}} \tag{3.4}$$

with

$V_{\mathrm{sl[S]}}$: volume of continental and global natural and agricultural soil [m^3];
$A_{\mathrm{[S]}}$: continental and global system area [m^2];
$fr\_A_{\mathrm{sl[S]}}$: area fraction continental and global natural and agricultural soil [-];
$h_{\mathrm{sl[S]}}$: depth continental and global natural and agricultural soil [m].

The FF is the same for ecotoxicity and human toxicity.

3.1.3. Exposure

The exposure factor (XF) determines the transfer of a chemical from an environmental media into humans and/or ecosystem system accordingly to different exposure pathways (Ferreira et al., 2019a).

As the fate factor, the exposure factor in a certain compartment is calculated by solving a set of mass balance equations (Fantke et al., 2017). The exposure factor expresses the accessibility for human or ecosystem contact (i.e. the fraction of the chemical dissolved in freshwater), represented by the fraction of the chemical transferred to the receptor population in a specific time period, such as a day (Fantke et al., 2015; Fantke et al., 2017).

For humans, an exposure model determines the XF, which describes the effective human intake of a specific environmental medium – air, water, soil – through routes inhalation and ingestion routes. For freshwater ecosystems, the XF dimensionless, applies only to the freshwater compartment, and expresses the fraction of the chemical within the freshwater compartment that is dissolved in water (Fantke et al., 2017).

3.1.3.1. Human exposure

The human exposure assessment of a chemical emitted into the environment (indoor or outdoor) is based on a cause-effect-chain connecting the (time-integrated) chemical mass in the environmental compartments (estimated in the fate model) to the substance intake by the total population via various exposure pathways (Rosenbaum et al., 2007).

Human exposure factors (XF_{human}) corresponding to specific pathways can be distinguished into direct exposure (direct consumption of an environmental in an environmental compartment such as drinking water, or inhalation of air) and indirect exposure factors (via food such as meat, dairy produce, vegetables, and fish) (Rosenbaum et al., 2007).

Each exposure pathway represents a contaminant transport mechanism from an environmental compartment into the human population. For indirect exposures, a food substrate can be contaminated in various environmental compartments. For example, a cow breathes air, drinks water, and eats forage (plants) and soil, any of which might contain a contaminant that can be subsequently transferred to the milk or meat obtained from that cow. Similar to fate factors that quantify the transfer from one environmental compartment to another, the exposure factors quantify the contaminant transferred from an environmental compartment into the human population via each exposure pathway (Fantke et al., 2017).

Therefore, the following exposure pathways are considered in the USEtox model:
- Inhalation of air,
- Ingestion of drinking water,
- Ingestion of meat and milk products,
- Ingestion of agricultural produce (distinguishing above-ground and below-ground),
- Ingestion of fish (distinguishing fresh water and coastal marine water fish).

3.1.3.2. Freshwater ecosystem exposure

The freshwater ecosystem exposure factor for an organic or inorganical chemical in freshwater is equal to the fraction of the chemical that is dissolved in this compartment (Brandes et al., 1996).

The size of the different metal species fractions varies among the different metals and also is also dependent on water chemistry parameters like pH and presence of anions and other cations (Fantke et al., 2017).

3.1.4. Effect

3.1.4.1. Human-toxicological effects

Effect factors for human toxicity (EF) are described separately for carcinogenic and non-carcinogenic effects, as well as data for effects after inhalation and oral exposure. A set of three human-health characterization factors can be reported, specifically "carcinogenic", "non-carcinogenic" and "total", of which the latter is the sum of carcinogenic and non-carcinogenic effects. The characterization factor for human toxicity impacts at midpoint level (human toxicity potential) is expressed in comparative toxic units (CTU_h), providing the estimated increase in morbidity in the total human population per unit mass of a contaminant emitted (cases/kg), assuming equal weighting between cancer and non-cancer effects due to a lack of more robust knowledge into this issue (Fantke et al., 2017).

3.1.4.2. Freshwater eco-toxicological effects

The ecotoxicity effect factor (EF) is calculated from ecotoxicity test results expressed as a concentration of dissolved chemical to which the organism is exposed in the test. It represents the chronic toxicity of the substance to a freshwater ecosystem (Brandes et al., 1996). The chronic toxicity is derived from observations on the sensitivities of a substance on the species of which an ecosystem can be composed (de Zwart, 2005).

The characterization factor for aquatic ecotoxicity impacts at midpoint level (ecotoxicity potential) is expressed in comparative toxic units (CTU_e) and provides an estimate of the potentially affected fraction of species (PAF) integrated over time and volume per unit mass of a chemical emitted ($PAF \cdot m^3 \cdot kg^{-1}$) (Fantke et al., 2017).

The interpellations explained above represent the use of USEtox to calculate characterization factors for human toxicity and freshwater ecotoxicity at midpoint level. The USEtox model results can be extended to determine endpoint effects expressed as disability adjusted life years (DALY) for human health impacts and potentially disappeared fraction of species (PDF) for ecotoxicological impacts (Fantke et al., 2017). In this thesis, midpoints level is considered because the reliability referent to these CFs is more robust and present a lower uncertainty than the endpoint CFs (Pfister & Hellweg, 2011). That is, the analysis will be done at the level of impacts (e.g. marine eutrophication) and not of damage (e.g. loss of marine biodiversity).

3.2. Description of the world regions in the USEtox and the site-specific parameters used for the selected regions

3.2.1. IMPACT World

Entities seeking to more comprehensively assess and mitigate the environmental health impacts of chemicals require a tool to quantify the impacts associated with global emissions, global supply chains and global food trade. To be effective, this tool needs to include the fate of the pollutant in multiple environments, cover multiple routes of exposure that represent the transfer of pollutants through food, and account for areas of high intensity exposure and cross-border transport, all while minimizing computational needs (Shaked, 2011).

This tool accuracy is increased while minimizing complexity by embedding a regionally-parameterized urban box to account for urban emissions and exposure in each region (Shaked, 2011). Trans-boundary pollutant transport can occur between regions through water flows and air flows. The regional divisions are based on a combination of politics (national boundaries), climate (latitudinal boundaries where global circulation changes), and population (for example, the densely-populated eastern part of China is separated from the rest of China) (Shaked, 2011).

IMPACT World divides the world into 17 subcontinental regions, 9 ocean regions and 33 coastal regions (Shaked, 2011) – Figure 3.3. As in previous IMPACT versions (Pennington et al., 2005), each continental region consists of an air zone (containing an air compartment) and a terrestrial zone (containing water, soil, vegetation, roots and sediments), and each oceanic region consists of an aerial zone and an ocean zone (containing surface oceans, deep oceans and ocean sediments). Each region is characterized by environmental and demographic parameters, such as rainfall rate, vegetation fraction and, most importantly for estimating population intake, vegetable and animal production intensity and population density (Shaked, 2011). IMPACT World was used to create and parameterize USEtox continents nested within a global box and analyse intra-continental variation on the sub-continental level. This is the only global interconnected-region model of pollutant fate and exposure modelling atmospheric air transport, whilst the only other interconnected global model GLOBOX (Sleeswijk and Heijungs, 2010) is based on average measured wind speeds at ground level (independent of direction) in capital cities. It models media-specific concentrations and intake fractions in the defined sub-continental regions fully interconnected by advective air and freshwater flows, which offers an interesting element of comparison with nested model, but results in an increased level of complexity (Kounina et al., 2014).

When compared to other models, IMPACT World put less emphasis on geographical boundaries and represent the best trade-off between continental or sub-continental resolution and the representation of population densities and meteorological conditions (Shaked, 2011).

With IMPACT World it is possible to examine the influence of surrounding region(s) on the fate and exposure of emissions within a considered sub-continent. One advantage of this model when compared to others is that this one explicitly connects the sub-continental zone to specific adjacent zones (Kounina et al., 2014).

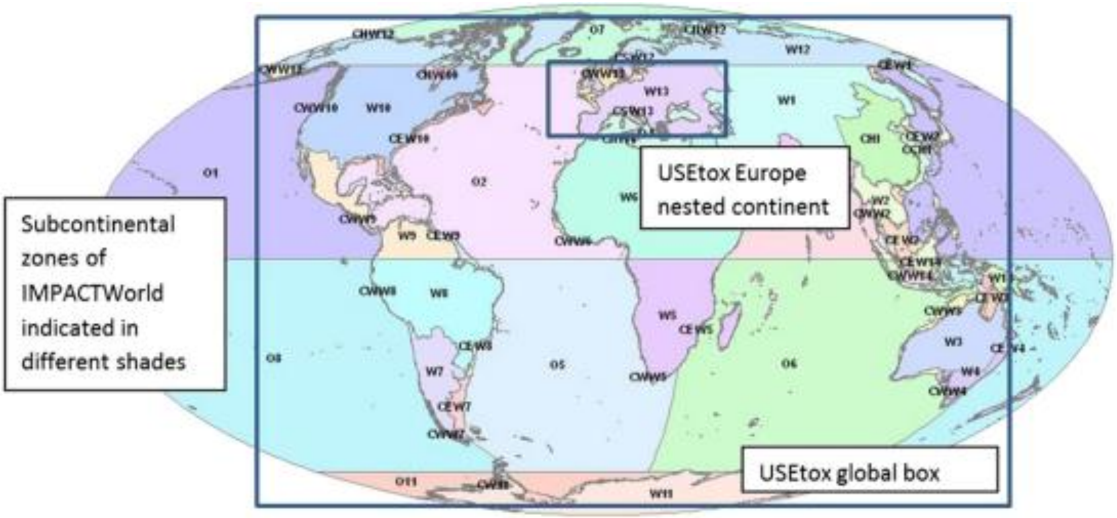

Figure 3.3. Depiction of how the IMPACT World model is used to parameterize the Europe box of USEtox, nested within the global box. Source: (Kounina et al., 2014.)

3.2.2. Choice of regions for evaluation

For comparative analysis, especially quantitative, of the characterization factors of different substances when emitted in different locations, 9 different regions of the world were selected for this purpose, including the USEtox default region. The regions for comparison, in the globe, described in the USEtox, are divided into continental regions and grouped continental regions, the latter being more all-encompassing. In Annex A, Table A1 presents all regions described in the model, all defined using specific parameter values, which assign individual characteristics to each region and will, therefore, be approached in the next subchapter. The nomenclature of the continental regions in the USEtox is done using the prefix "W", followed by the identification number of each region (e.g. the W1 region refers to Central Asia). The grouped continental regions involve several of the ones described above (e.g. the grouped region of Oceania includes the continental regions W3 – Northern Australia and W4 – Southern Australia and New Zealand), and their nomenclature is done with full name, these are the regions described last in Table A1.

Given the large number of regions described in USEtox, its complete analysis would already exceed the interests of this study. Therefore, in the selection of continental regions of study, in an attempt to cover a wide diversity of areas of the globe, while selecting a reasonable number of regions, individual and grouped continental regions were selected (four of each), and also the USEtox default region to comparation of results. The main objective of this choice was to have a diverse area of study, in order to obtain a good comparability of results of substance characterization factors and, thus, to get weighted conclusions from a diverse database. Taking this into account, the selected regions were:

- Europe - **W13**;
- Northern Europe and Northern Canada – **W12**;
- Central Asia - **W1**;
- USA and Southern Canada - **W10**;
- Southeast Asia - **Grouped Continental Region**;
- Oceania - **Grouped Continental Region**;
- Africa - **Grouped Continental Region**;
- Latin America - **Grouped Continental Region**
- USEtox Default Region – **USEtox Default**

Individual continental regions include Europe (includes much of the continent with the exception of the Northern part); Northern Europe and Northern Canada (includes all Northern European countries and Northern parts of Canada); Central Asia (includes all countries in Central Asia and also Southeast China); the U.S. and Southern Canada (includes Southern Canada and the entire U.S. region except Alaska).

The grouped continental regions include Southeast Asia, Oceania, Africa and the Latin American region. Southeast Asia includes the W2 region (Indochina, includes all countries on the Indochinese Peninsula), the W14 region (includes all Pacific and Eastern Indian islands, e.g. Indonesia and American Samoa), and also India, China and Japan. Oceania includes the W3 region (includes Northern Australia and the islands of Wallis and Futuna) and the W4 region (includes South Australia and New Zealand). Africa includes the W5 (South Africa) and W6 (North, East, West and Central African) region. Latin America includes the W7 region (Argentina+, includes Argentina and surrounding countries), the W8 region (Brazil+, includes Brazil and surrounding countries) and the W9 region (includes all Central American countries and Caribbean islands, e.g. Cuba and Dominica). The representation of these zones on the map can be seen in Figure 3.3. This way, much of the continental land area is represented in the model, with the choice of only 8 study areas, a number that allows to explore in more detail each one of these regions.

3.2.3. Obtaining method of each site-specific parameter

This section is dedicated to the analysis of how each site-specific parameter is obtained and understanding its values. The site-specific parameters of USEtox are defined on a continental scale, on a global scale, on an urban scale, for the human population, exposure and intake rates based on production. The site-specific parameters described by USEtox to define each region are represented in Table A2 to Table A6.

Continental scale

Starting with the site-specific parameters defined on the continental scale. The areas of each region (including land area, maritime area) and fractions of area (freshwater, natural soil, agricultural soil and other soils) were obtained using GIS (Geographic Information Systems). According to esri (https://www.esri.com/en-us/what-is-gis/overview), this program consists of a system of hardware, software, spatial information, computational procedures and human resources that allows and facilitates the analysis, management or representation of geographic information. Fractions of agricultural land and other soils have the same value for all regions. This result is due to the fact that the fraction of natural soil area corresponds to almost 90% of the total area in all regions, and therefore the fraction of agricultural soil area was assumed to be 10% for all regions, with the remaining area (around 2%) being the corresponding to freshwater and other types of soil. The freshwater area fraction is obtained based on GIS computation for IMPACT World.

The fraction of agricultural soil area is assumed to be 10% for all regions; and the fraction of natural soil area is calculated using the formula (Shaked, 2011):

$$areafrac_{nat\ soil} = 1 - areafrac_{agr\ soil} - areafrac_{freshwater} - areafrac_{other\ soil} \quad (3.5)$$

It is important to mention that the land area is defined as being the area of land, including areas of natural soil, agricultural soil, freshwater and urban area. The maritime area is defined as the coastal area.

Some site-specific parameters are quantified with a standard value (value used for the default USEtox region). This is due to the fact that there are limitations inherent in the model as a result of simplifications (Shaked, 2011). These limitations will be addressed in detail in the next subchapter. Thus, the temperature is assumed to have a default value for all regions of 12ºC.

Advective rate constants between regions are obtained using horizontal wind speeds from GEOS-Chem, a global tropospheric chemistry model that provides averages of 6 hours of wind speed from the Goddard Earth Observeing System (2005) at 2°×2.5° resolution, represented in Figure 3.4. The components north, south, east and west of wind speeds are arithmetic averages, temporally over a year, vertically over the three lowest atmospheric layers in GEOS-Chem (corresponding to 800 m high) and horizontally over the continental boundaries (Shaked, 2011). Selecting the value of this parameter also has associated limitations, which will be covered in the next subchapter. Therefore, the value of 3 m/s for the wind speed on the surface of all regions was assumed. The resolution is defined as a cartesian grid (latitude-longitude), which is chosen according to the desired accuracy (Vaníček, 2003). For example, the “thinner” the resolution, the more accurate the results obtained will be because the study area is divided into more subspaces where parameters are obtained and compared separately.

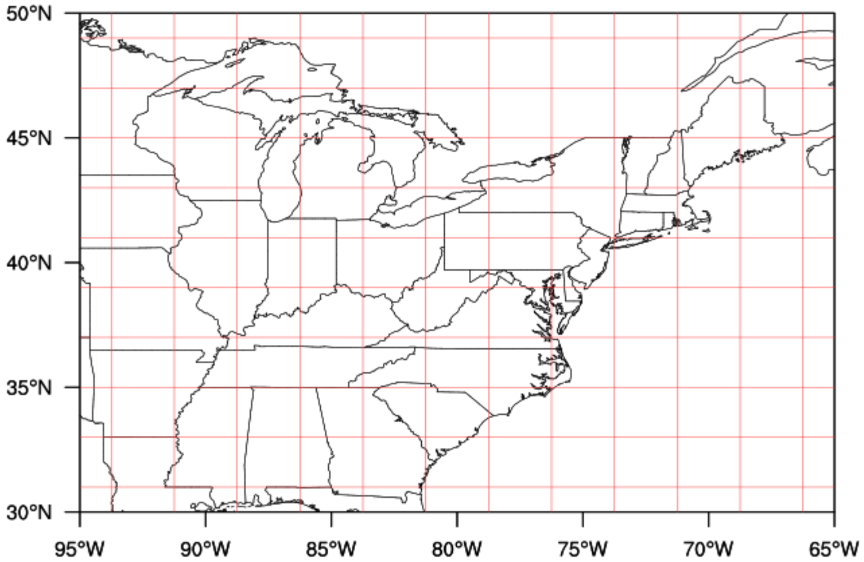

Figure 3.4. Detail of GEOS-Chem 2°x2.5° grid over USA. Source: Wiki-seas (http://wiki.seas.harvard.edu/geos-chem/index.php/GEOS-Chem_horizontal_grids).

As described in ksfire (https://www.ksfire.org/environment), the mixing height is defined as the height above the surface along which a pollutant can be dispersed. As done in previous impact assessment models, atmospheric transport was defined using an air layer with a mixing height of 800 m (Hofstetter, 1998). This is an estimate commonly used in life cycle impact assessment, including the USEtox model. The wind speed over the mixing height (m/s) is dependent on parameters such as the mixing height (m) and the effective dilution rate (m^2/s), which is a product of the first two. Since the dilution rate has the same value for all regions, 610 m^2/s (which is the harmonic average of twice-daily measurements in 75 US urban areas) (Marshall et al., 2005), the wind speed over mixing height decreases with increasing mixing height. Therefore, the value of this speed is variable regionally. For example, the US region has an average wind speed of 7.0 m/s above the lowest 1000 meters of air (Kounina et al., 2014).

The rain rate, as well as the depth of freshwater, are defined based on GIS computing for IMPACT World.

The value of the freshwater discharge fraction, this is, the average river flow on the continental/global scale, is obtained from the standard landscape data and is assumed to be 0 for all regions due to the characteristics of the model, for water mass balance purposes.

The Minnesota Pollution Control Agency (https://www.pca.state.mn.us/) explains that the runoff fraction is defined as the flow fraction of each watershed divided by precipitation for this watershed. It is the proportion of precipitation that does not infiltrate and is not assumed by evapotranspiration, and thus ends up as escape. This parameter is defined based on GIS computing for IMPACT World.

The infiltration fraction is the fraction of the flow of water that goes from aboveground into the subsurface (Huffman et al., 2013). Its value is obtained from the standard landscape data and is assumed to be 26.9% for all regions.

Soil erosion is the denudation of the upper soil layer. It is a form of soil degradation. This natural process is caused by the dynamic activity of erosive agents, for instance water, ice (glaciers), snow, air (wind), plants and animals (including humans), according to Ontario Ministry of Agriculture Food and Rural Affairs (http://omafra.gov.on.ca/english/engineer/facts/12-053.htm). Its value is obtained from the standard landscape data and is assumed to be 0.03 mm.yr^{-1} for all regions.

Irrigation is the artificial application of water to soil through various systems of pipes, pumps and sprays. Irrigation is generally used in areas where precipitation is irregular or is expected to dry out, as described in Centers for Disease Control and Prevention (https://www.cdc.gov/healthywater/other/agricultural/types.html). This value is obtained using AQUASTAT, which provides information on water use by sector, as well as water use for irrigation purposes, for each region.

It is important to note that the parameters obtained using GIS, AQUASTAT or other models/programs, are not empirical or estimated. These values are obtained from reliable data. Otherwise, the parameters assumed due to lack of information are of uncertain value which can result in greater uncertainty when using them. In this case, a value set as the default for USEtox is used, so that it is an allowable value for all regions, thus resulting in less uncertainty.

Global scale

All the parameters mentioned above are now redefined on a global scale, with some nuances. All areas and fractions of area obtained for the continental scale are now redefined to a global scale taking into account continental landscape data.

The remaining parameters are assumed to have a value equal to that assumed for the standard value used for the landscape data of the USEtox model, for the continental scale.

Urban Scale

All parameters on the urban scale are assumed to have a value equal to that assumed for the standard value of USEtox, that is, the land area, and the fractions of populated and unpopulated area.

Human Population

The parameters for the human population (global, continental and urban) are redefined based on the data of parameters at the continental level. For the human population parameter in urban areas/areas, data for more than 3500 urban areas (covering 2.2 billion people) are provided by the United Nations and the World Bank (Angel et al., 2005; UN, 2008), and properties in smaller urban areas are estimated based on region-specific regressions between populations and population density (Shaked, 2011).

Exposure

The parameters related to exposure (human respiration rate and water intake) are assumed as typical values used as standard values for USEtox and are the same for all regions. Human respiration rate = 13 m^3/(person*day); water intake = 14 l/(person*day).

Production-based intake rates

Production-based intake rates are divided into several parameters, which characterize the various routes that the substance in study can take before being consumed directly or indirectly by humans. All these parameters are defined for a global scale and for a continental scale and the former are obtained through recalculation based on continental data. The second, for agricultural production, meat and dairy products, are obtained from FAO (Food and Agriculture Organization) production data from 2001; in the case of freshwater and coastal marine waters fish, result from data from FAO FishSTAT, the FAO universal software for statistical fishing time series.

A summary of how site-specific parameters are defined on continental scale and production-based intake rates is presented in Table 3.1 and Table 3.2, respectively. The remaining parameters defined in USEtox are either assumed to be the default value defined by the model or are redefined based on continental-scale parameter values.

As already referred, many of the mentioned parameters are assumed to be the same as the default value described by USEtox – Table 3.3. This simplification is due to the fact that, the LCIA often does not have a specific location for emissions, and therefore may depend on standard values for landscape and meteorology (Bare, 2006). To conclude, the default data of the site-specific parameters of USEtox are obtained to mitigate errors when compared with the obtaining of parameters in specific regions. Therefore, typical values are used that approach reality in that location.

Table 3.1. Site-specific parameters obtaining method on continental scale.

PARAMETER	OBTAINING METHOD
AREAS	GIS computation
TEMPERATURE	Default value
WIND SPEED	GEOS-Chem
PRECIPITATION AND FRESHWATER DEPTH	GIS computation
FRESHWATER DISCHARGE FRACTION	Default value
RUN OFF FRACTION	GIS computation
INFILTRATION FRACTION	GIS computation
SOIL EROSION	Default value
IRRIGATION	AQUASTAT

Table 3.2. Obtaining method for production-based intake rate parameters.

PARAMETER	OBTAINING METHOD
AGRICULTURAL PRODUCTION, MEAT AND DAIRY PRODUCTS	FAO
FRESHWATER AND COASTAL MARINE WATERS FISH	FAO FishSTAT

Table 3.3. Site-specific parameters that are equal for all regions in the USEtox model. Adapted from: (Ferreira et al., 2019b).

PARAMETER	VALUES	UNIT
TEMPERATURE	1.20E+01	°C
SURFACE WIND SPEED	3.00E+00	m s^{-1}
SOIL EROSION	3.00E-02	mm yr^{-1}
HUMAN BREATHING RATE	1.30E+01	m^3/person day
WATER INGESTION	1.40E+00	l/person day

3.3. Study limitations associated with data/model

As mentioned in the previous subchapter, the obtaining of some parameters is done taking into account inherent limitations, which often results in simplifications (Shaked, 2011). Another common situation is the adoption of standard values defined by USEtox, when information on certain parameters is scarce or has associated uncertainty.

In the definition of temperature, the assumption of a permanent regime requires constant emissions and constant transport rates between different regions and environments, which, for example, neglects the daytime, seasonal and annual variations in emissions, winds and temperatures (Shaked, 2011). Hence the value of 12ºC for the surface temperature of all regions.

For wind speed, to conserve mass, air flows are balanced so that the total flows in and out of each region are equal. Since atmospheric flows vary very vertically, daytime, seasonally and annually, these averages do not fully capture atmospheric transport processes, but are intended to provide a better approximation of cross-border transport as well as provide a framework for future refinements (Shaked, 2011). Thus, the value of 3 m/s was assumed for the wind speed on the surface of all regions.

For the parameter of the air mixing height, no other overall average mixing height was available, especially in view of the need to take into account the transport of pollutants through mixing heights varying in time and spatial currents; future work should determine the best mixing height for such application (Shaked, 2011)

Because the relevant dependencies are non-linear, the effective dilution rate is not simply a product of arithmetic averages of the wind speed and mixing height. So, was used the best available value of a dilution rate of 610 m^2/s, which is the harmonic average of twice-daily measurements in 75 US urban areas (Marshall et al., 2005).

About freshwater discharge fraction, IMPACT World flows are advective flows based on river discharges out of the subcontinental zone (Global Runoff Data Centre, 2002), while USEtox uses a water balance approach based on precipitation, evapotranspiration, infiltration and runoff (Kounina et al., 2014).

Finally, in the definition of exposure parameters (human respiration rate and water intake), the limitation is that water intake is not constant worldwide (e.g. in certain areas of Africa, water intake per person per day is lower than the European average). For simplification and to provide a framework for future refinements, where the evaluation of parameters for specific sites can be taken into account, a constant value for water intake was assumed.

3.4. Sensitivity analysis to site-specific parameters

Using the USEtox model, a sensitivity analysis to site-specific parameters of each region was performed, whose main objective is to understand the influence they have on the behaviour of substances, once released into the environment, and how this varies the value of the substance characterization factors. To accomplish this task, parameter values with various orders of magnitude were varied, in order to have an "artificial region", where one can draw conclusions about the influence on the variation of the value of these parameters.

This variation was made to all parameters which are significant in the results presented in the following chapter, only including those that vary depending on the region. Parameters were taken into account on the continental scale, well as the parameter related to the human population and production based-intake rates. Thus, with variation of several parameters, a vast database is obtained, and more concise conclusions can be drawn about the influence of the value of site-specific parameters on the characterization factors of substances, using the USEtox model.

All site-specific parameters are presented in Annex A, respectively from Table A2 to Table A6.

3.5. Selection of substances to be analysed

In the context of the comparison of human and environmental toxicological characterization factors associated with substance emissions in different regions of the world, using the USEtox model, five substances were selected for analysis: Formaldehyde; allyl alcohol; n-octane; lead and dioctyl terephthalate. The substances were defined only with the data whose information was available, so there are substances with more quantified data than others, hence there are some flagged as "interim" for the calculation of characterization factors (this happens when the level of uncertainty in the calculation is considerable). All parameters related to the characterization of the substances introduced in the model for the calculation of the toxicological characterization factors are shown in Annex B – Table B1.

A brief description of each type of chemical selected is presented. Formaldehyde is a volatile organic compound made from methanol, a highly toxic alcohol; allyl alcohol is an organic compound. Like many alcohols, it is a water-soluble, colorless liquid, and is more toxic than typical small alcohols; n-octane is a hydrocarbon and an alkane (organic compound). When inhaled it may cause irritation of respiratory tract, depression, and pulmonary edema (Sung et al., 2010); lead (II) is a compound characteristic of the inorganic chemistry of lead. It is a heavy metal that is denser than most common materials. Because of its mass and malleability, lead has long been the primary metal used for ammunition, but it is an extraordinary toxic element. The chemical properties of lead and its harmful effects on humans have been known nearly since the discovery of this element. Exposure of humans to lead occurs by several routes including ingestion of contaminated food (animals shot using lead ammunitions), lead poisoning of waterbirds due to ingestion of spent lead gunshot and others (Knott et al., 2010); dioctyl terephthalate is an organic compound and a non-phthalate plasticizer.

These five substances have been selected primarily to cover a wide range of substances with different types and different behaviours when released into the environment. In this way, it is possible to draw more informative conclusions about the influence not only of the type of environment in which the chemicals are released, but also of the nature of the substances.

4. RESULTS AND DISCUSSION

The substance characterization factors of substances on human health (cancer and non-cancer effects) and ecosystems were calculated by employing the USEtox model. Beyond the default scenario used by the USEtox model, eight different regions were selected to understand the potential influence of the site-specific conditions to the characterization factors of substances. In this chapter, the results obtained for the characterization factors with the USEtox model for each region, are presented and discussed. The characterization factors were calculated for the five substances selected, considering a direct emission into the air or the natural soil. The analysis of the results obtained with this procedure also permits to identify the contributors to the fate and exposure fractions in order to understand the variations for the different regions. It is important to mention that the effect factor does not vary for the different regions as the toxicity is not dependent of the site-specific conditions; however, the effect factor can influence the potential toxicological impact.

4.1. Analysis and interpretation of USEtox results for the selected regions

The results of the characterization factors are analyzed for the fate, intake and effect factors, for an emission to the rural air and to the natural soil.

4.1.1. Fate factors

Firstly, the comparison of the total FF (sum of the FF values of all compartments) of the five selected substances associated with the different emission regions assessed with the USEtox model, is analyzed. Then, the distribution of each substance in the different compartments is described in detail, to understand the different behaviour that the substances can present when emitted in different regions with different site-specific parameters.

Table 4.1 presents the fate factor (FF) assessed for five substances, in each of the previously selected regions, considering an emissions into rural air. From this table one can draw general conclusions about FF variations in different regions and which are more significant. Considering the same region (e.g. Europe), it is observed that the only inorganic substance under analysis, lead, has a higher FF value than the other substances (up to five orders of higher magnitude). This is due to the high value presented by the partition coefficients of this substance, specifically between solid particles and water (k_p). This high value of k_p results in a low polarity of lead, therefore a greater ease of mixing with soil, for example, resulting in a greater persistence in this compartment. Another reason is that this substance has lower degradation coefficients in all compartments, thus indicating a high persistence of lead in the compartment where it is deposited. Dioctyl terephthalate has the lowest FF values, which is then the substance with the least persistence globally, in a given deposition compartment. This is justified by the fact that this substance has high degradation coefficients, in particular in air ($kdeg_A$), and in water ($kdeg_W$), in relation to the other substances, resulting in a lower persistence in these compartments (and a lower FF value). The remaining three substances, formaldehyde, allyl alcohol and octane, present intermediate values of FF.

Comparing the total FF values in different regions, it is concluded that these do not have a significant variation - the difference is below an order of magnitude. From these results, it can be assumed that a given substance will have a similar overall persistence regardless of the region where it is emitted. Despite this, there are compartments where substances persist more than others and, in this part, local parameters pose an important role in determining results. This subject will be discussed in detail from Figure 4.1 to Figure 4.5. The FF values presented for the USEtox default region vary little from those presented for the selected regions.

Table 4.1. Fate Factors assessed for five substances considering different regions, for an emission into continental air.

		Total
	Zone	**Fate Factor**
Formaldehyde	Europe	**7.44E+00**
	Northern Europe & Northern Canada	**8.29E+00**
	Central Asia	**5.61E+00**
	Southeast Asia	**9.33E+00**
	Oceania	**8.66E+00**
	Africa	**5.41E+00**
	USA & Southern Canada	**7.34E+00**
	Latin America	**8.46E+00**
	Default USEtox	**7.10E+00**
	Europe	**2.10E+00**
	Northern Europe & Northern Canada	**2.49E+00**
	Central Asia	**1.41E+00**

Allyl alcohol	Southeast Asia	**2.58E+00**
	Oceania	**2.42E+00**
	Africa	**1.33E+00**
	USA & Southern Canada	**1.92E+00**
	Latin America	**2.00E+00**
	Default USEtox	**1.82E+00**
n-octane	Europe	**1.78E+00**
	Northern Europe & Northern Canada	**1.78E+00**
	Central Asia	**1.78E+00**
	Southeast Asia	**1.78E+00**
	Oceania	**1.78E+00**
	Africa	**1.78E+00**
	USA & Southern Canada	**1.78E+00**
	Latin America	**1.78E+00**
	Default USEtox	**1.78E+00**
Lead	Europe	**1.70E+05**
	Northern Europe & Northern Canada	**1.32E+05**
	Central Asia	**2.15E+05**
	Southeast Asia	**7.43E+04**
	Oceania	**9.59E+04**
	Africa	**2.32E+05**
	USA & Southern Canada	**1.24E+05**
	Latin America	**6.90E+04**
	Default USEtox	**1.49E+05**
Dioctyl terephthalate	Europe	**6.45E-01**
	Northern Europe & Northern Canada	**6.29E-01**
	Central Asia	**6.68E-01**
	Southeast Asia	**6.32E-01**
	Oceania	**6.37E-01**
	Africa	**6.73E-01**
	USA & Southern Canada	**6.53E-01**
	Latin America	**6.57E-01**
	Default USEtox	**6.55E-01**

Figure 4.1 to Figure 4.5 shows the distribution of an emission into rural air for the other compartments associated with formaldehyde, allyl alcohol, octane, lead and dioctyl terephthalate, respectively. The differences in total FF values do not vary significantly for the different regions. Nevertheless, there are substances with more significant differences

than others considering different emission compartments – for instance, octane has a FF value of 1.78E+00 days regardless of the emission region; whilst lead has a FF of 2.32E+05 days when released on the African continent and a FF of 6.90E+04 days when released in the Latin American region.

The results presented for octane are justified by the fact that this substance has a Henry Law Coefficient (K_{H25C}) much higher than the other substances under analysis. This coefficient, also called the air-water partition coefficient, relates the concentration of a chemical in air over its concentration in water. Since octane is an insoluble substance in water, this coefficient indicates that this substance will disperse almost entirely into the air and, therefore, this is the compartment where this substance persists the most, regardless of the emission region. In the case of the difference of FF in a lead emission, is due to the local parameters of the emission regions. The fact that the African continent has a large amount of land area, will favor the deposition in soil compartments, and as lead, as explained earlier, tends to deposit in this compartment, this will result in the higher value of FF in this region. But what is contributing, on a larger scale, to this result, is not the land area but the rain rate. Since this rate is higher in the Latin American region when compared to the African continent (1.61E+03 and 5.08E+02 mm.yr^{-1}, respectively), this results in greater degradation and a lower persistence of lead in the soil. Also, the transport of lead by the action of rain to other compartments, where the persistence of this substance is lower, contributes to this result. Therefore, a lower FF value associated with the Latin American region is observed.

Analyzing each region in detail, it is observed that there are more persistent substances in some compartments than in others, due to their physical-chemical characteristics, as well as the site-specific parameters of the region. In Figure 4.1 it can be observed that formaldehyde has a higher persistence in seawater, than the other substances (it is also observable a considerable contribution of this compartment on a global scale, to the total value of FF). These results are mainly due to the fact that this substance has a low coefficient of degradation in water ($kdeg_W$) compared to those presented in other compartments. This substance does not tend to be deposited in the remaining compartments, so present a reduced FF value in these compartments. It is important to note that although seawater on the continental scale is the main deposition compartment of this substance, this does not happen in all regions, and for the regions of the African continent and Central Asia, this compartment presents a small contribution to the value of the total FF, as will be analyzed later.

Figure 4.2 shows that allyl alcohol exhibits a similar behaviour to formaldehyde in terms of persistence and inter-compartment transfer (they present the same value for $kdeg_W$).

Octane, in Figure 4.3, is only visible a deposition/transfer compartment, this being the air (mainly on the continental scale, but also visible on the global scale), which justification was mentioned before.

Taking into account the physical-chemical characteristics of lead, this substance tends to deposit in the natural soil, with persistence values higher than those of the other substances, as mentioned earlier (Figure 4.4).

Finally, the main deposition compartment of dioctyl terephthalate is in air, although it is also transferred for the natural soil, as shown in Figure 4.5. The high value of K_{H25C} of this substance (lower than octane, but higher than the other substances), results in a high persistence in the air. As well as the low coefficients of degradation in the soil (lower than all substances except lead), they give an intermediate persistence value to this substance in this compartment.

It is also important to mention the difference in FF values in each compartment, for the same substance in different regions. This is mainly due to the site-specific parameters of each region, which attribute these differences. For instance, analyzing an emission of formaldehyde into rural air, if the transfer is for seawater compartment, the FF is noticeably higher in Southeast Asia when compared to the African continent or Central Asia (Figure 4.1). This is mainly due to the fact that the continental area of Southeast Asia has a much larger sea area than the African continent and Central Asia, facilitating the deposition in this compartment. In addition, the rain rate is also quite higher in Southeast Asia, revealing this an important parameter for the value of FF in aquatic compartments. The same is observed with an emission of allyl alcohol (Figure 4.2). Otherwise, analyzing a lead emission, in natural soil the FF is much higher on the African continent when compared to the Southeast Asian region, as can be seen in Figure 4.4. The justification for this result has been given before and is mainly related with the highest rain rate presented in Southeast Asia, compared to the African continent. The fact that the latter also has a larger land area, favors the deposition of lead in this compartment.

Finally, analyzing Figure 4.6, corresponding to the persistence of lead in the natural soil, the main deposition compartment of this substance. Although the FF of lead in this compartment presents higher values in several orders of magnitude in comparison with the FF of the other substances, the difference of its persistence between regions does not reach an order of magnitude. These variations correspond only to the parameters of each region, and how site-specific parameters are quantified.

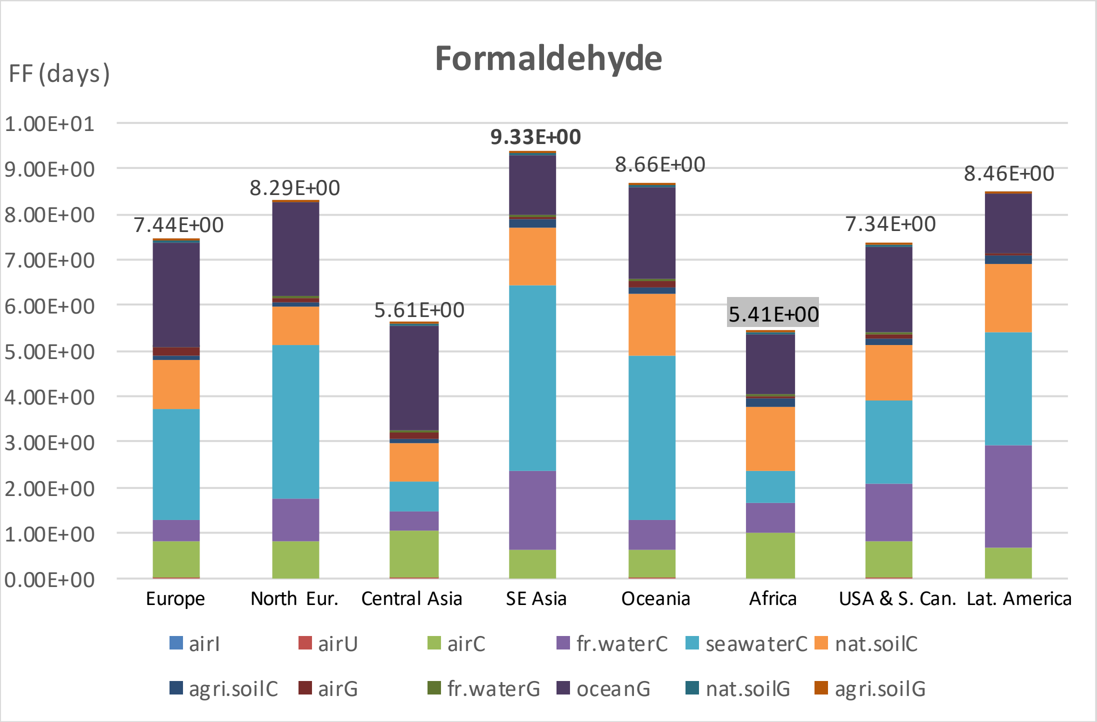

Figure 4.1. Comparison of the distribution of a direct emission of formaldehyde into rural air for the other compartments, considering the different regions.

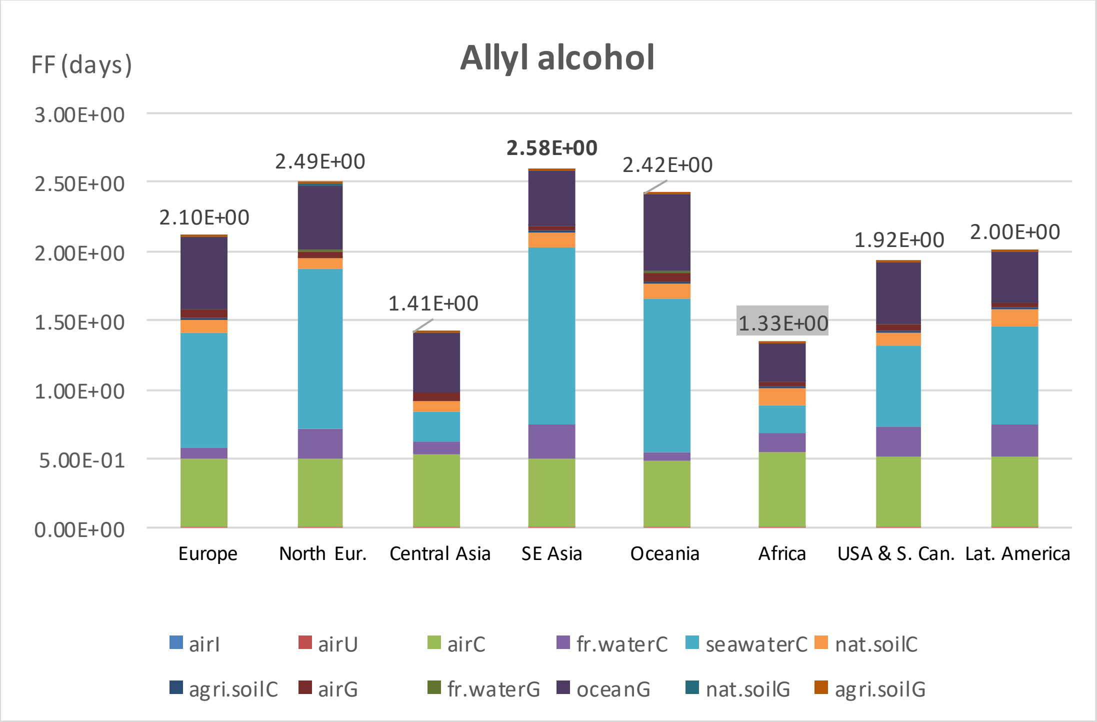

Figure 4.2. Comparison of the distribution of a direct emission of allyl alcohol into rural air for the other compartments, considering the different regions.

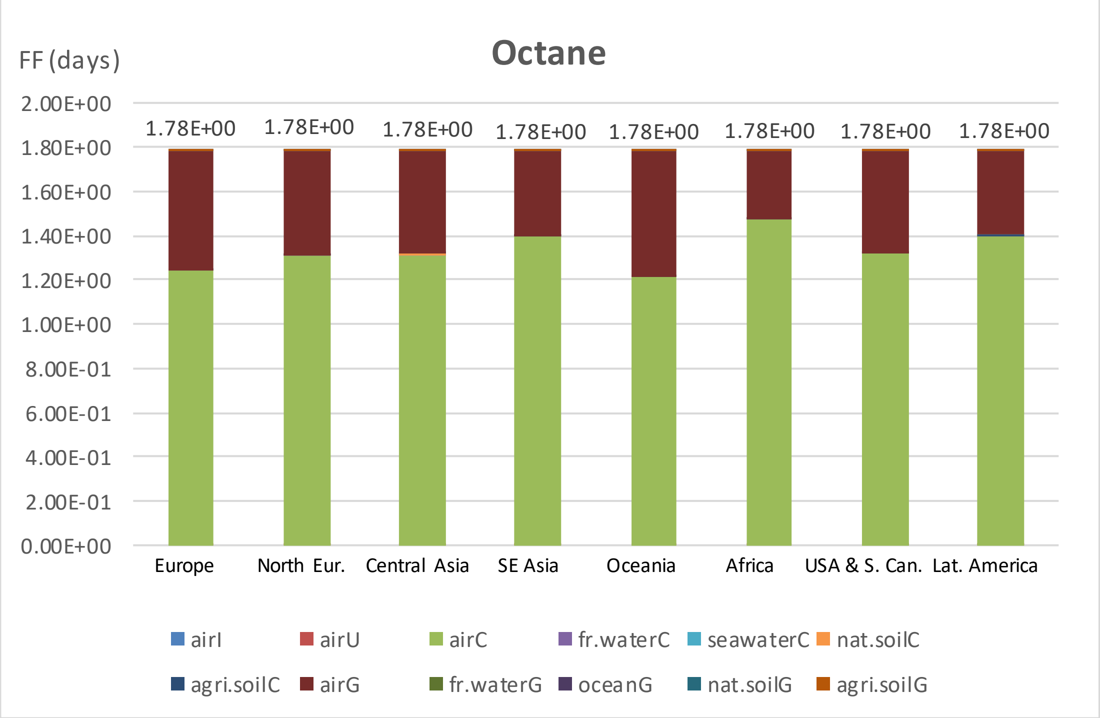

Figure 4.3. Comparison of the distribution of a direct emission of octane into rural air for the other compartments, considering the different regions.

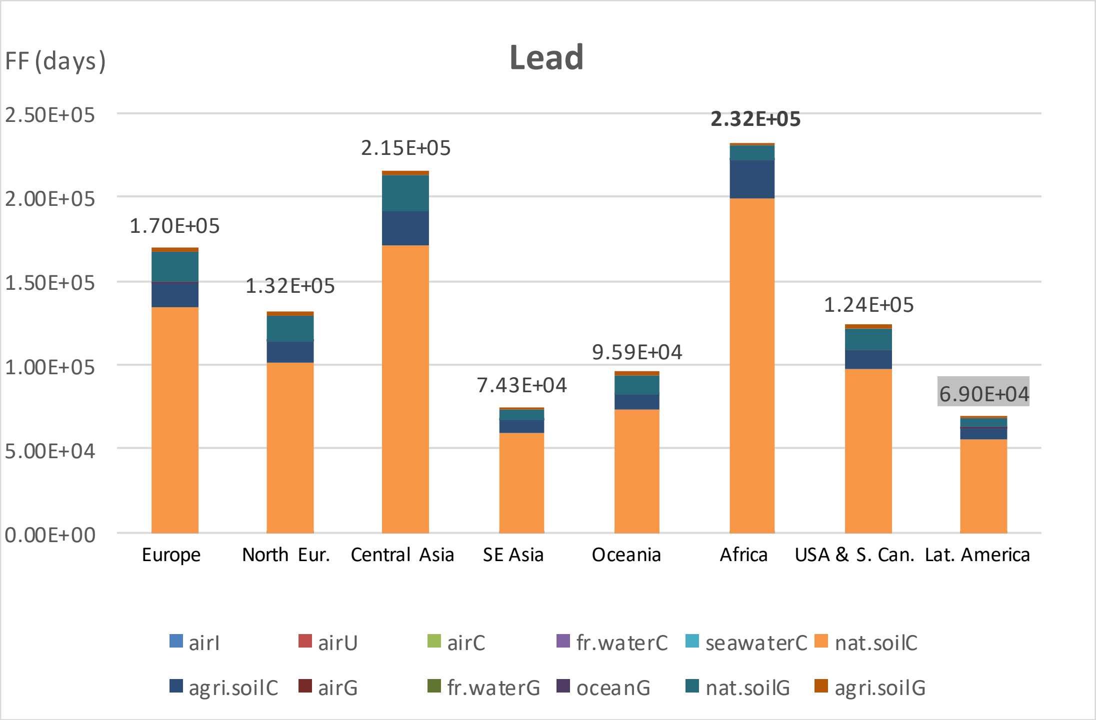

Figure 4.4. Comparison of the distribution of a direct emission of lead into rural air for the other compartments, considering the different regions.

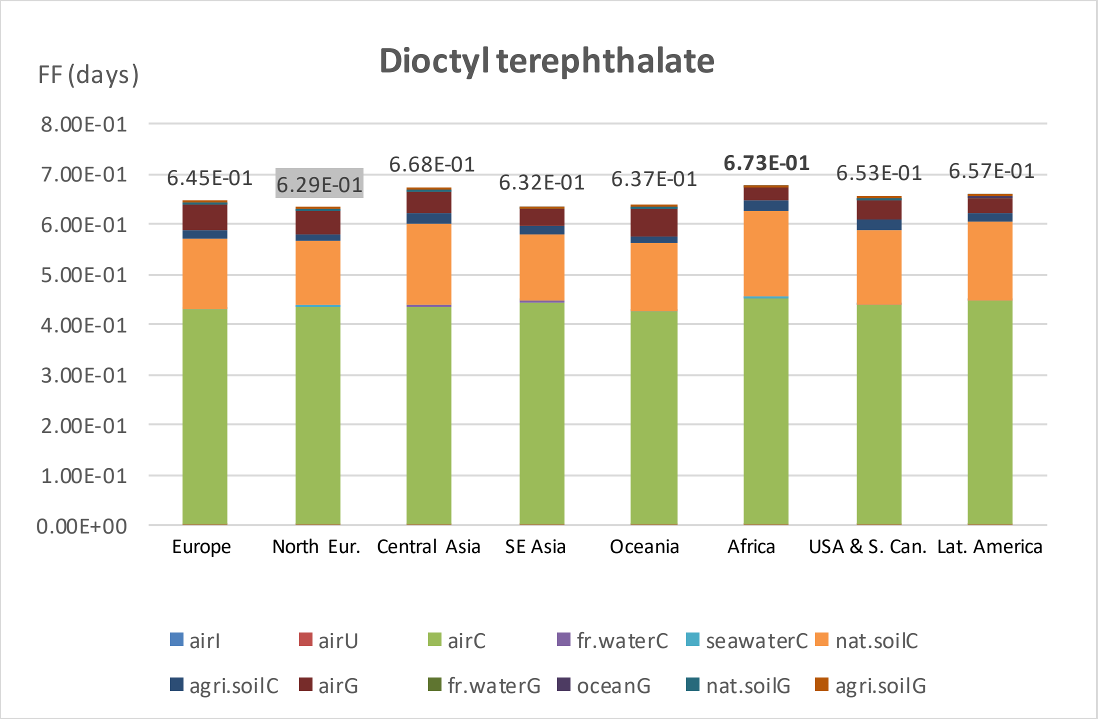

Figure 4.5. Comparison of the distribution of a direct emission of dioctyl terephthalate into rural air for the other compartments, considering the different regions.

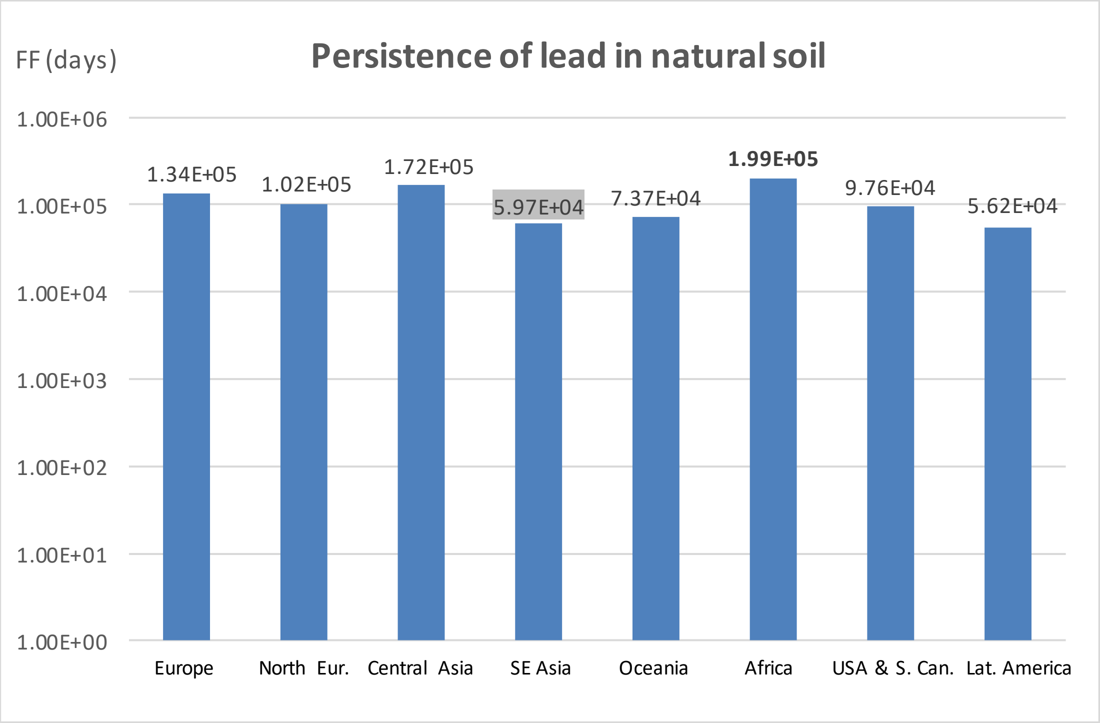

Figure 4.6. Comparison of the Fate Factor of lead in natural soil in different locations, considering an emission into continental rural air.

Analyzing now the results for an emission in natural soil presented in Table 4.2. Initially comparing with the FF resulting from an emission to the rural air, it can be concluded that the FF values of formaldehyde, octane and lead remain similar, so these substances have a similar overall persistence in the environment, regardless of whether their emission occurs in rural air or in natural soil. Allyl alcohol and dioctyl terephthalate does not have the same behaviour, as they present significant differences in the total FF values. Respectively, the first presents FF values more than one order of magnitude higher (e.g. for an emission of allyl alcohol in rural air on the African continent, the total FF value is 1.33E+00 days, while the same emission released in natural soil in the same region, the total FF value is 1.75E+01 days). Dioctyl terephthalate, presents total FF values to almost two orders of magnitude higher when compared to an emission in the rural air (e.g. for an emission of dioctyl terephthalate in the rural air on the European continent, the total FF value is 6.45E-01 days, while if this emission is released in natural soil in the same region, this value is 5.49+01 days), then indicating a greater persistence when released into natural soil. These results are due to the fact that the compartments where some substances persist most are different, as will be presented in Figure 4.7 to Figure 4.11, with the respective dispersion between the compartments of the selected substances.

Comparing the FF values for the emission of a substance, but in different regions, such as in an emission for rural air, it is concluded that they do not have a significant variation (i.e. the difference is bellow an order of magnitude). Therefore, a given substance will potentially have a similar overall persistence regardless of the region where it is emitted. As in the previous case, there are compartments where substances persist more than others and, in this part, site-specific parameters pose an important role in determining the results.

As in the case of an emission for rural air, the FF values presented for the USEtox default region do not have significant variations when compared to those presented for the selected regions.

Table 4.2. Fate Factors assessed for five substances considering different regions, for an emission into continental natural soil.

		Total
	Zone	**Fate Factor**
	Europe	**8.50E+00**
	Northern Europe & Northern Canada	**9.35E+00**
	Central Asia	**8.94E+00**
	Southeast Asia	**9.48E+00**

Formaldehyde	Oceania	**8.71E+00**
	Africa	**8.36E+00**
	USA & Southern Canada	**9.54E+00**
	Latin America	**1.04E+01**
	Default USEtox	**8.94E+00**
Allyl alcohol	Europe	**1.71E+01**
	Northern Europe & Northern Canada	**1.83E+01**
	Central Asia	**2.14E+01**
	Southeast Asia	**1.28E+01**
	Oceania	**1.23E+01**
	Africa	**1.75E+01**
	USA & Southern Canada	**1.65E+01**
	Latin America	**1.34E+01**
	Default USEtox	**1.56E+01**
n-octane	Europe	**5.69E+00**
	Northern Europe & Northern Canada	**5.69E+00**
	Central Asia	**5.69E+00**
	Southeast Asia	**5.69E+00**
	Oceania	**5.69E+00**
	Africa	**5.69E+00**
	USA & Southern Canada	**5.69E+00**
	Latin America	**5.69E+00**
	Default USEtox	**5.69E+00**
Lead	Europe	**2.95E+05**
	Northern Europe & Northern Canada	**2.46E+05**
	Central Asia	**4.00E+05**
	Southeast Asia	**1.07E+05**
	Oceania	**1.41E+05**
	Africa	**3.10E+05**
	USA & Southern Canada	**1.80E+05**
	Latin America	**8.43E+04**
	Default USEtox	**2.22E+05**
Dioctyl terephthalate	Europe	**5.49E+01**
	Northern Europe & Northern Canada	**5.49E+01**
	Central Asia	**5.49E+01**
	Southeast Asia	**5.49E+01**
	Oceania	**5.49E+01**
	Africa	**5.49E+01**

	USA & Southern Canada	**5.49E+01**
	Latin America	**5.49E+01**
	Default USEtox	**5.49E+01**

Analysing now Figure 4.7 to Figure 4.11 with the respective dispersion between the compartments of the substances selected for all regions and using the same methodology as in an emission for rural air. For the different regions the differences in total FF values do not vary significantly, since between different regions the same substance has a FF value with differences lower than an order of magnitude, when released into the environment.

Also analyzing the value of FF between different substances, taking into account the same region, lead, as in the case of an emission into rural air has a higher persistence value (up to almost five orders of magnitude) than the remaining four substances under analysis, as presented in Figure 4.10. This result is justified by the high persistence of this substance in the soil.

Of the four organic substances analyzed, the highest values of FF, in the case of an emission to the natural soil, are now presented by dioctyl terephthalate (value of 5.49E+01 days for all regions - Figure 4.11), indicating a greater global persistence in the environment of this substance, in comparison with the others. Otherwise, octane is the least persistent substance in all selected regions, being this the one with the lowest FF values (5.69E+00 days for all regions - Figure 4.9). In the case of dioctyl terephthalate, the result is due to this substance presenting degradation coefficients in the soil lower than the other three organic substances and, in the case of an emission to the natural soil, this results in a higher FF value. In the case of octane, being this a substance that persists in the air as demonstrated in the previous case, when the emission to the natural soil is released, it results in a smaller total FF of this substance. Formaldehyde, allyl alcohol and dioctyl terephthalate present intermediate persistence values, with slight differences between regions.

An emission into the natural soil presents also different behaviour for the transfers between the different compartments, as observed for the case of an emission into air. It is concluded that for an emission to the natural soil, the rate of migration of the substance to other compartments is lower when compared to an emission to the rural air. This is because when released into natural soil the substance tends to deposit; while when it is released into the rural air, the substances tend to disperse more easily to other compartments by the action of wind and rain.

For example, looking at the case of an emission of formaldehyde and allyl alcohol, presented in Figure 4.7 and Figure 4.8 it is also noticeable that these substances persist in part in freshwater, although it is a very small part when compared to the value of FF in natural soil. Only in the Latin American region there is a greater persistence of these two substances in freshwater, compared to natural soil. These differences are due to the site-specific parameters of each region, as explained earlier, due to a higher rain rate, the region of Latin America, will favor the persistence of these substances in aquatic compartments, even if the emission is released in the soil. The fact that Latin America region has a high runoff fraction, this is the proportion of precipitation that does not infiltrate, also favors the persistence of these substances in aquatic compartments.

A similar behaviour is observed for octane, that is a higher volatile substance, so it tends to disperse into the rural air, as can be seen in the Figure 4.9, although, it is an insignificant part when compared to the FF value in natural soil.

Finally, lead and dioctyl terephthalate when released into the natural soil tend to be deposited in this compartment in its entirety, as can be observed by the value of FF presented in this compartment in Figure 4.10 and Figure 4.11. This is due to the characteristics of these substances, already presented above, and also to the emission being released in natural soil.

The difference in FF values in each compartment for the same substance in different regions is mainly due to the site-specific parameters of each region, which attribute these differences. Analyzing a lead emission in natural soil, in this compartment the FF is noticeably higher in Central Asia, when compared to the Latin American region, where although the difference does not reach an order of magnitude, it reaches close values, as in the case of an emission for rural air, as shown in Figure 4.10. These differences are related with parameters such as land area and rain rate, as in the case of an emission to the rural air. The same happens for an emission of allyl alcohol, presented in Figure 4.8.

Finally, looking at Figure 4.12, corresponding to the persistence of lead in natural soil, the main deposition compartment of this substance. Although the FF of lead in this compartment presents higher values in several orders of magnitude in relation to the FF of the other substances, the difference of its persistence between regions does not reach an order of magnitude. These variations correspond only to the parameters of each region, and how local parameters are quantified.

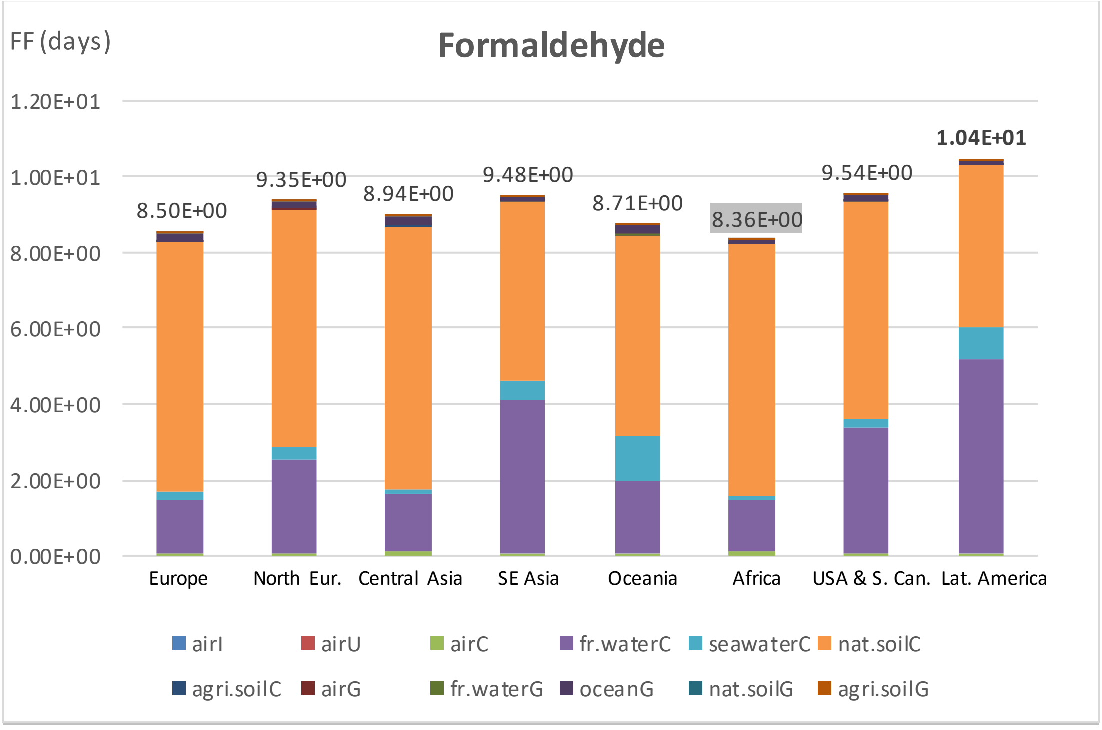

Figure 4.7. Comparison of the distribution of a direct emission of formaldehyde into natural soil for the other compartments, considering the different regions.

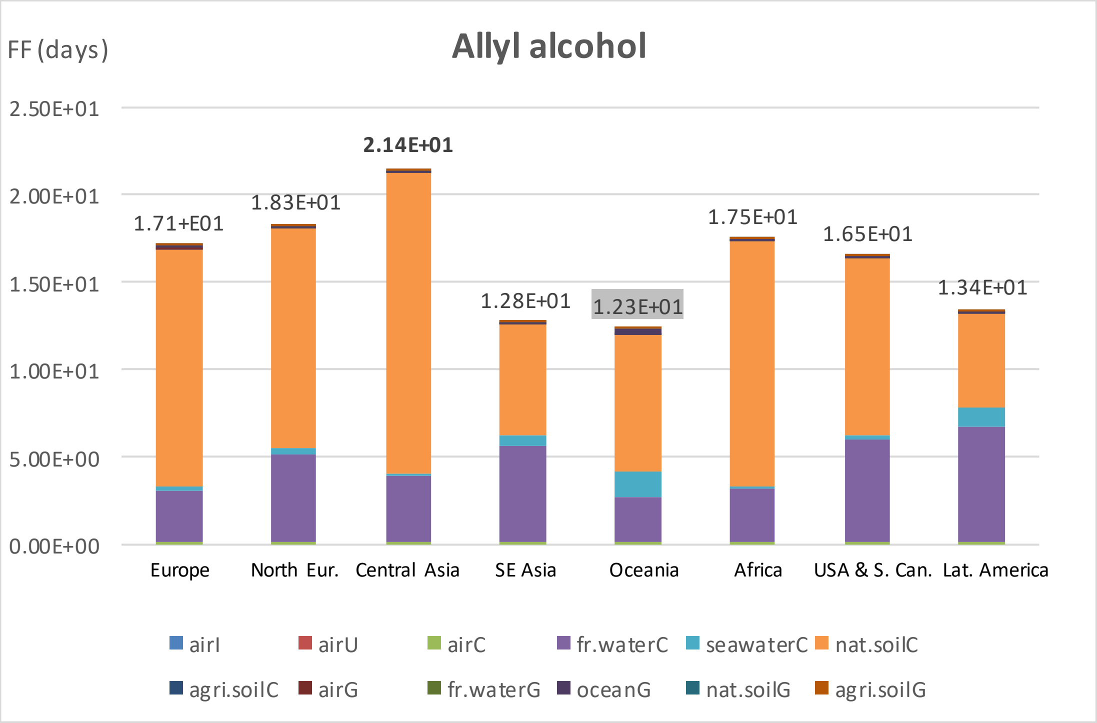

Figure 4.8. Comparison of the distribution of a direct emission of allyl alcohol into natural soil for the other compartments, considering the different regions.

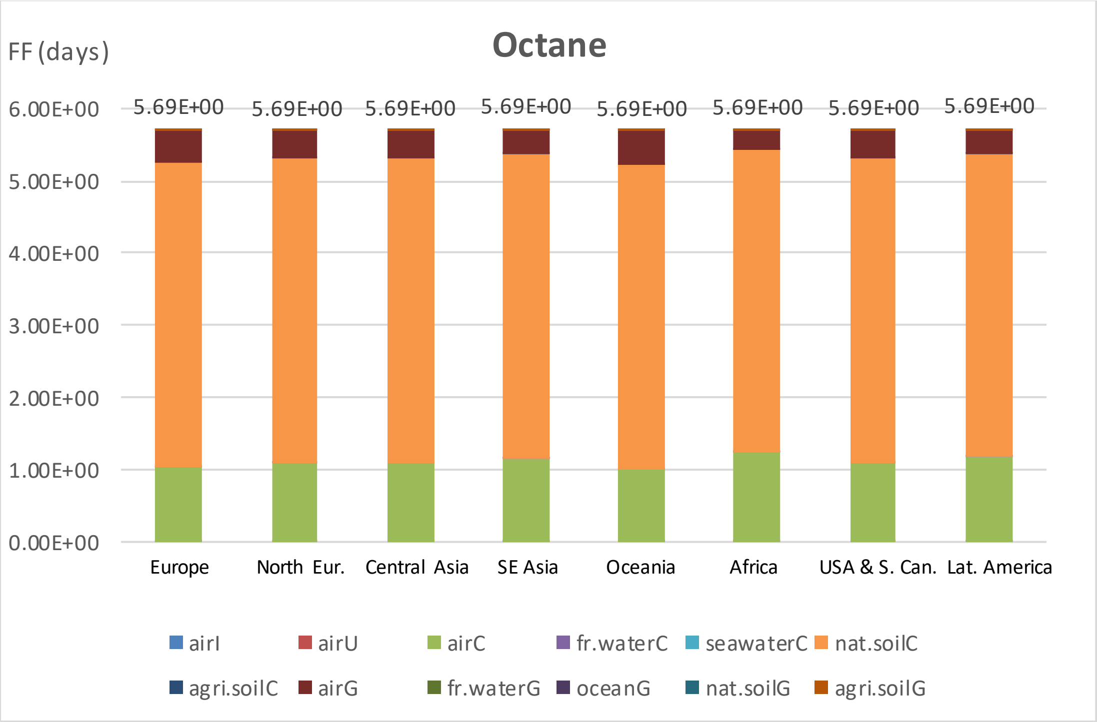

Figure 4.9. Comparison of the distribution of a direct emission of octane into natural soil for the other compartments, considering the different regions.

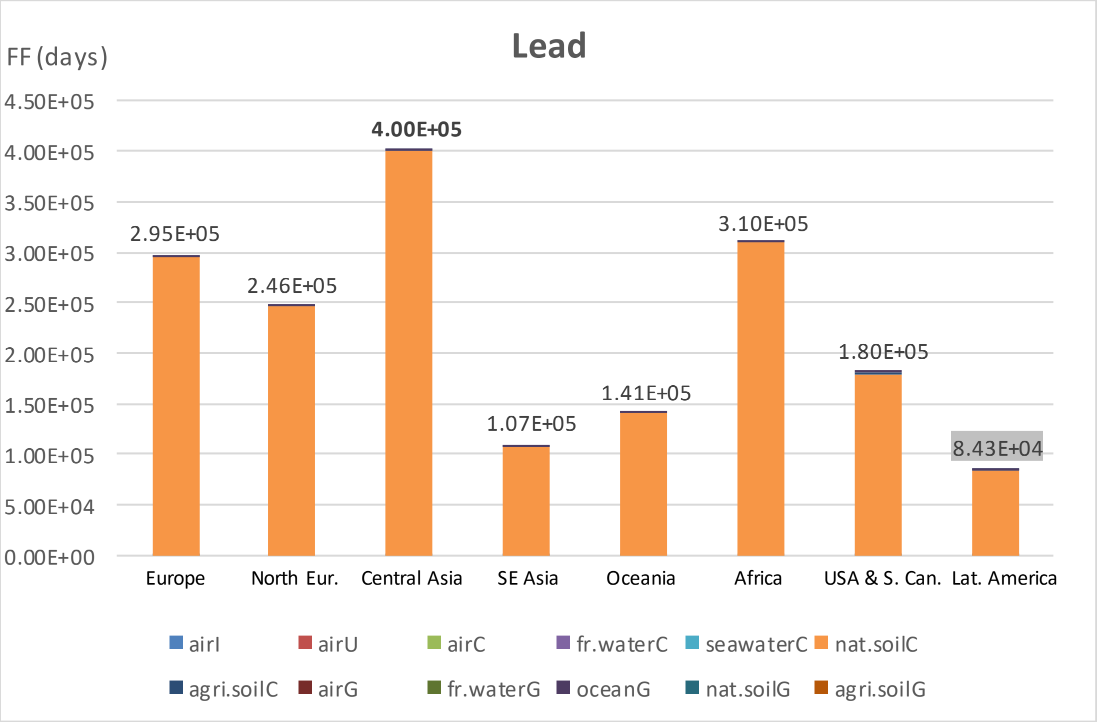

Figure 4.10. Comparison of the distribution of a direct emission of lead into natural soil for the other compartments, considering the different regions.

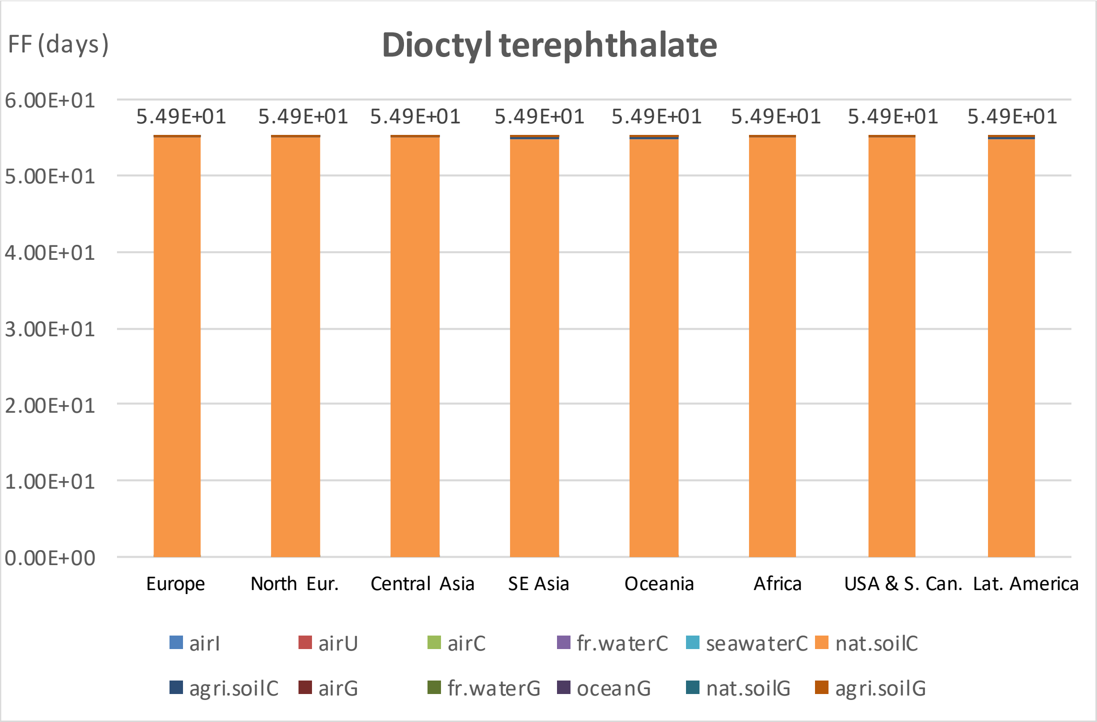

Figure 4.11. Comparison of the distribution of a direct emission of dioctyl terephthalate into natural soil for the other compartments, considering the different regions.

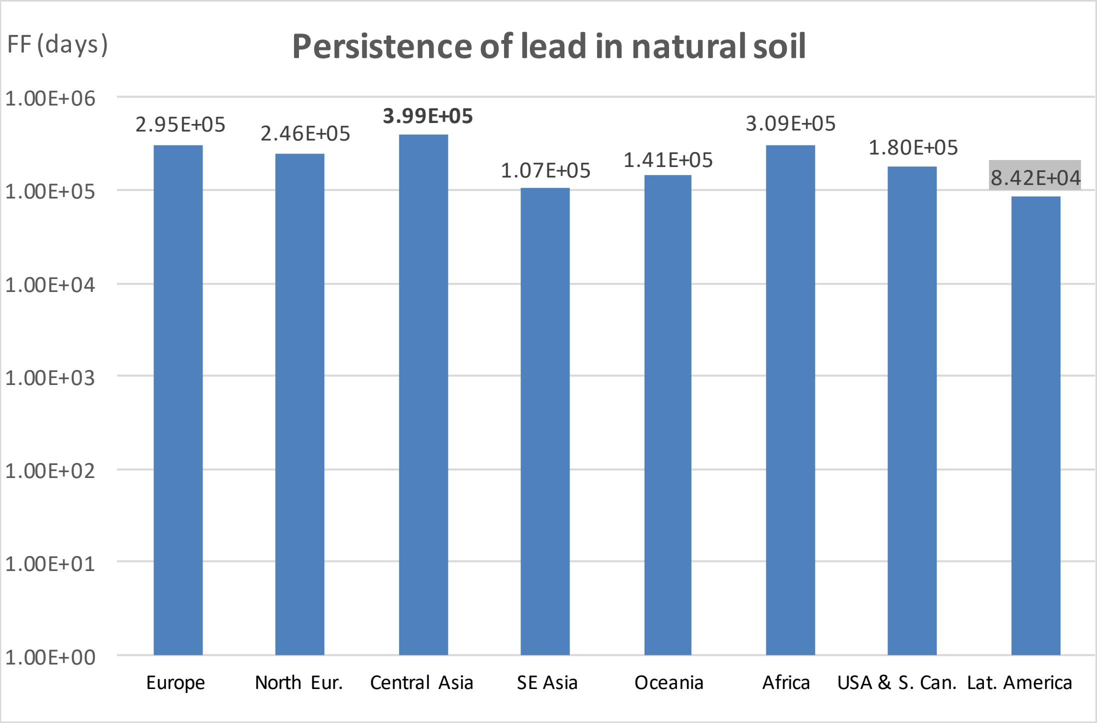

Figure 4.12. Comparison of the Fate Factor of lead in natural soil in different locations considering an emission into continental natural soil.

4.1.2. Intake factors

In the analysis of the results of the intake factors, were analyzed an emission to rural air and another to natural soil. Firstly, it is analyzed the total iF values of inhalation and ingestion pathways of each substance, for all the selected regions. Then, the analysis of iF was performed, for the same region and between regions, for the specific pathways of exposure by ingestion, in order to understand the influence that site-specific parameters have on these values. With the presentation of the results with the contributions of each intake route in Figure 4.18 to Figure 4.23, more detailed conclusions can be drawn, such as on which intake route, a person is more susceptible to the consumption of a given substance and in which regions is most likely to be exposed to that substance.

Figure 4.13 to Figure 4.17 presents the comparison of the total intake by ingestion and inhalation for the different regions. From these graphs, general conclusions can be drawn about the variations in iF. It is concluded that the site-specific parameters of each region pose an important role in the calculation of the iF of a given substance. It can be observed in that, by selecting a substance, both inhalation and ingestion iF vary at least one order of magnitude between regions. For instance, considering a formaldehyde emission to rural air in Southeast Asia, results in an inhalation iF of 1.40E-06 kg intake/kg emitted, while if that emission is released in Oceania, the iF value is 4.55E-08 kg intake/kg emitted, a substantially lower value, as shown in Figure 4.13. This means that although the amount of a substance emitted is the same, there are regions where humans will be more susceptible to the exposure of certain substances, resulting from the site-specific parameters of the emission region, especially population and production based-intake rates that involve parameters such as the eating habits of the population and consumption of products from production above and below ground. The characteristics of the substances are also necessary to take into account in the analysis as they define the most likely deposition compartment of that substance and therefore also influence the value presented for the iF in a given region.

Looking at the iF values between different substances one can also conclude which are most likely to be present the different intake routes (inhalation or ingestion). For instance, Figure 4.16 shows that lead is a substance that is mostly deposited in the soil, so it is more likely to have a higher exposure to humans by ingestion than by inhalation; on the contrary, octane has higher inhalation iF values when compared to those for ingestion, as presented in

Figure 4.15. Justified by the example presented earlier, the highest iF values are those associated with the lead ingestion route.

The iF values presented in Table 4.3 to Table 4.7, for the USEtox default region, correspond to intermediate iF values of the selected regions, both in the inhalation and ingestion routes.

Figure 4.18 to Figure 4.23 show, as a percentage, the presence of each one of the selected substances on the different routes of exposure, for each region.

Analyzing each substance separately, in Figure 4.18 it is concluded that formaldehyde is more likely to be intaked on the ingestion route than in the inhalation route, since the ingestion iF are higher than those of inhalation for all regions. The main route of ingestion of this substance is above-ground production, reaching the highest iF value for an emission in Southeast Asia (much higher value when compared to an emission in Northern Europe, for example). This is result of the high bioaccumulation factor value from air gas phase to above ground produce of formaldehyde when emitted in the air, which confers a high exposure factor to this substance in this exposure pathway. Although the consumption of products derived from above-ground production is higher in Northern Europe, the value of the iF associated with this intake route is higher in Southeast Asia due to the much larger population in the latter region. Only in the Latin American region a higher iF of this substance related to below-ground production compared to above-ground production is observed. And this is due to the fact that the Latin American region has higher consumption of products from below-ground production compared to above-ground production, unlike the other selected regions.

Allyl alcohol has different intake routes, depending on the region considered, as can be seen in Figure 4.19. For example, when considering an emission of this substance in Central Asia, the inhalation route is most likely to occur, however, if this emission is released in the USA and South Canada, the most likely intake route is due to above-ground production. Since the emission is released in the rural air, and due to the nature of this substance, the inhalation route has a considerable iF value, despite this, the high consumption of above-ground production products in the USA and South Canada region makes the iF of allyl alcohol superior in this intake route in this region.

Despite the emission region, octane has a uniform behaviour regarding the most likely intake route, and it is undoubtedly the inhalation route, due to the physical and chemical characteristics of this substance, shown in Figure 4.20. As explained in the previous subchapter, for an emission to rural air, this substance tends to persist mainly in the air, thus resulting in a high inhalation iF value and negligible iF values in the remaining intake pathways. It should also be noted that although the inhalation route is dominant in this substance, the emission region also poses an important role in the amount that is actually intaked from this pollutant, since there are discrepancies in the iF values (e.g. the inhalation iF corresponding to an emission in Southeast Asia is 3.03E-06 kg intake/kg emitted, while for an emission in Northern Europe is 1.03E-07 kg intake/kg emitted). Again, in this case, this difference in values is due to the fact that the Southeast Asian region has a larger population.

Lead has as main intake route in all regions, the above-ground production, but in Latin America is observed a high intake fraction of this substance related to the production below ground, as previously justified and presented in Figure 4.21. Despite discrepancies in the values of lead iF, this difference does not reach an order of magnitude between different regions.

Finally, dioctyl terephthalate presents above-ground production as its main intake route, but in some regions such as Oceania, dairy products consumption constitutes an important fraction of the total iF value of intake of this substance, as presented in Figure 4.22. This is result of the high bioaccumulation factor value from air gas phase to above ground produce of dioctyl terephthalate when emitted into the air. The result of this substance iF in Oceania is due to the fact that the consumption of dairy products in this region is much higher than the others and therefore results in greater exposure of the population to this substance on this intake route. In this case, the emission region strongly influences the amount that is effectively consumed from dioctyl terephthalate when an emission occurs in the rural air. For instance, the ingestion iF associated with this emission in Europe is 1.11E-04 kg intake/kg emitted, while if it is released in Northern Europe, it is 1.96E-06 kg intake/kg emitted, constituting a difference of almost two orders of magnitude. Since the consumption of products from above-ground production has a negligible difference between these two regions, the difference in iF values is due to population differences, as in the situations described above (a larger population corresponds to a higher iF value).

Analyzing the results of Figure 4.23, corresponding to the intake pathway distribution of all substances in USEtox default region, these present values common to most regions presented in the previous graphs.

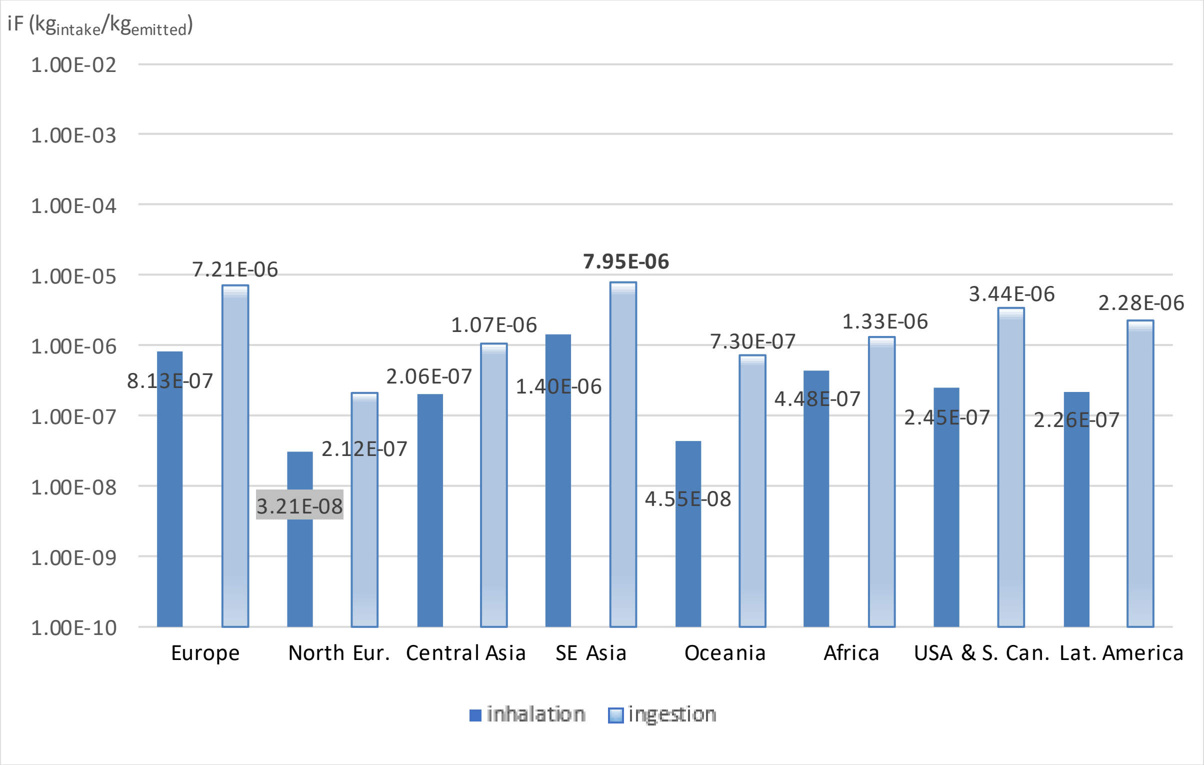

Figure 4.13. Comparison of the intake Factor of formaldehyde in different regions for inhalation and ingestion (emission into continental rural air).

Table 4.3. Intake Factor of formaldehyde in USEtox default region for inhalation and ingestion (emission into continental rural air).

Substance	**Intake Factor** **Zone**	Inhalation	Ingestion
Formaldehyde	USEtox default region	**1.08E-06**	**7.72E-06**

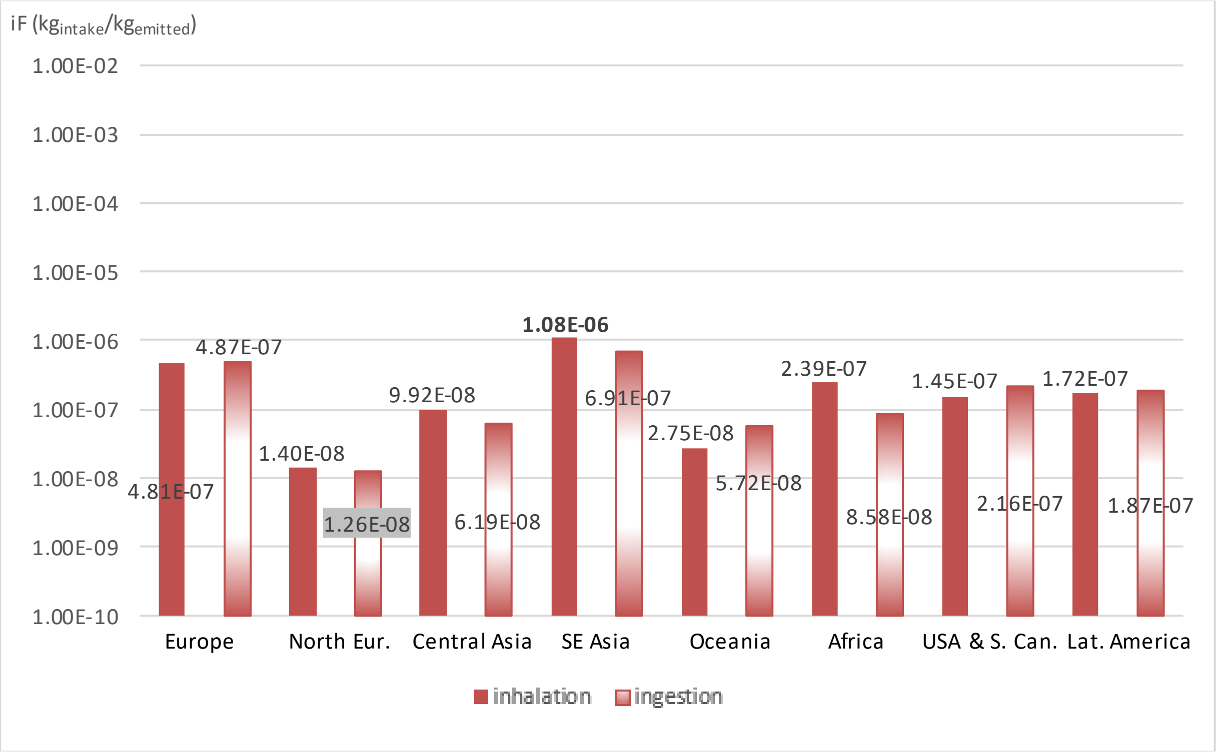

Figure 4.14. Comparison of the intake Factor of allyl alcohol in different regions for inhalation and ingestion (emission into continental rural air).

Table 4.4. Intake Factor of allyl alcohol in USEtox default region for inhalation and ingestion (emission into continental rural air).

Substance	**Intake Factor** **Zone**	Inhalation	Ingestion
Allyl alcohol	USEtox default region	**6.62E-07**	**6.58E-07**

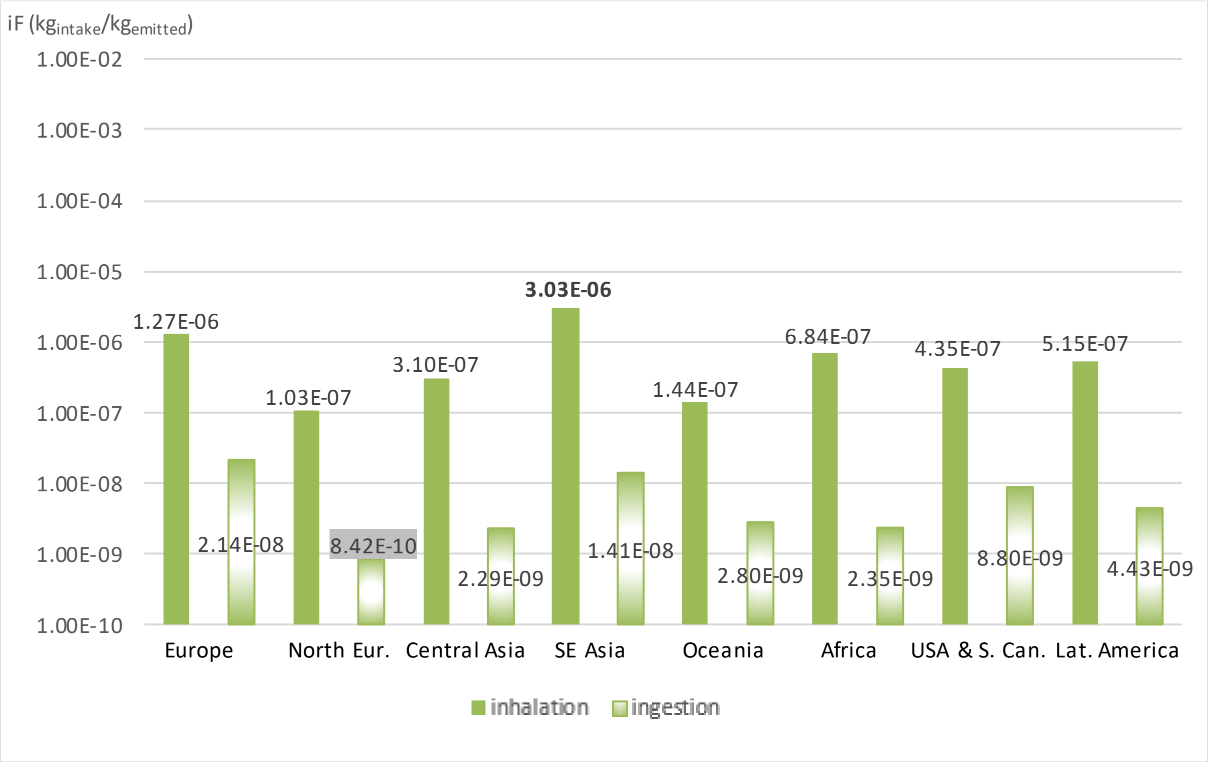

Figure 4.15. Comparison of the intake Factor of octane in different regions for inhalation and ingestion (emission into continental rural air).

Table 4.5. Intake Factor of octane in USEtox default region for inhalation and ingestion (emission into continental rural air).

Substance	**Intake Factor** **Zone**	Inhalation	Ingestion
Octane	USEtox default region	**1.71E-06**	**1.25E-08**

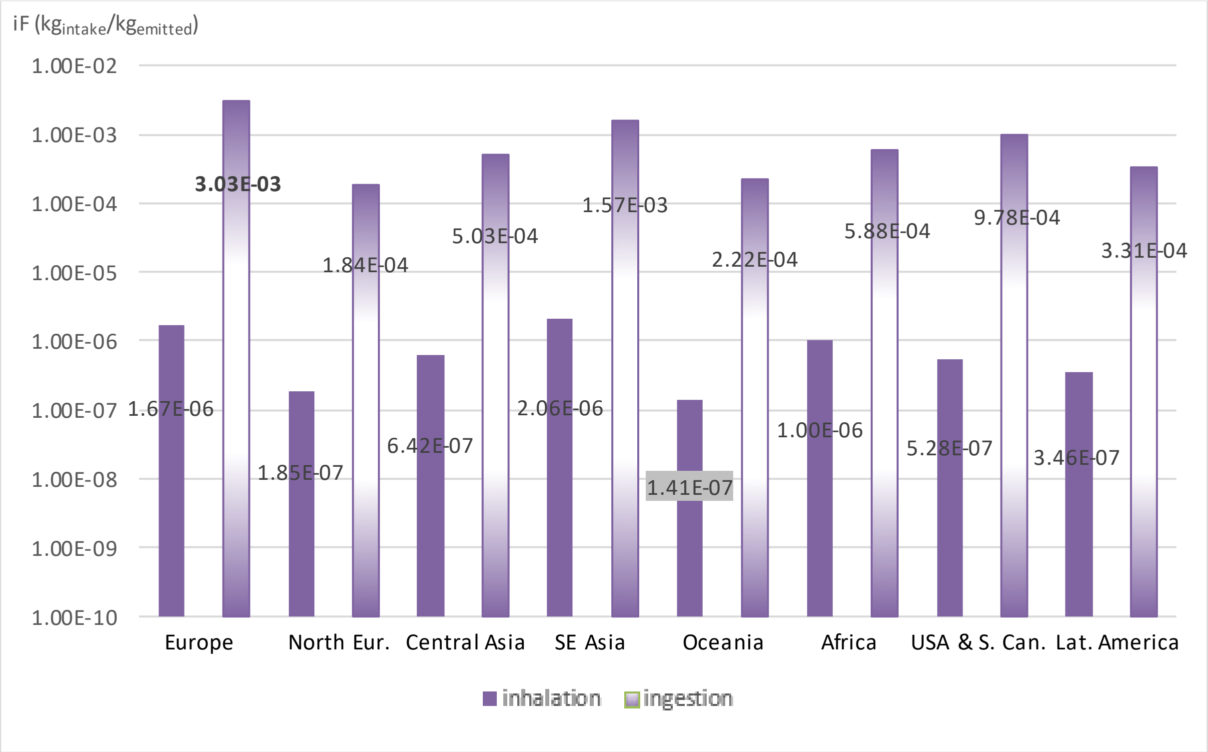

Figure 4.16. Comparison of the intake Factor of lead in different regions for inhalation and ingestion (emission into continental rural air).

Table 4.6. Intake Factor of lead in USEtox default region for inhalation and ingestion (emission into continental rural air).

Substance	**Intake Factor** **Zone**	Inhalation	Ingestion
Lead	USEtox default region	**1.98E-06**	**1.91E-03**

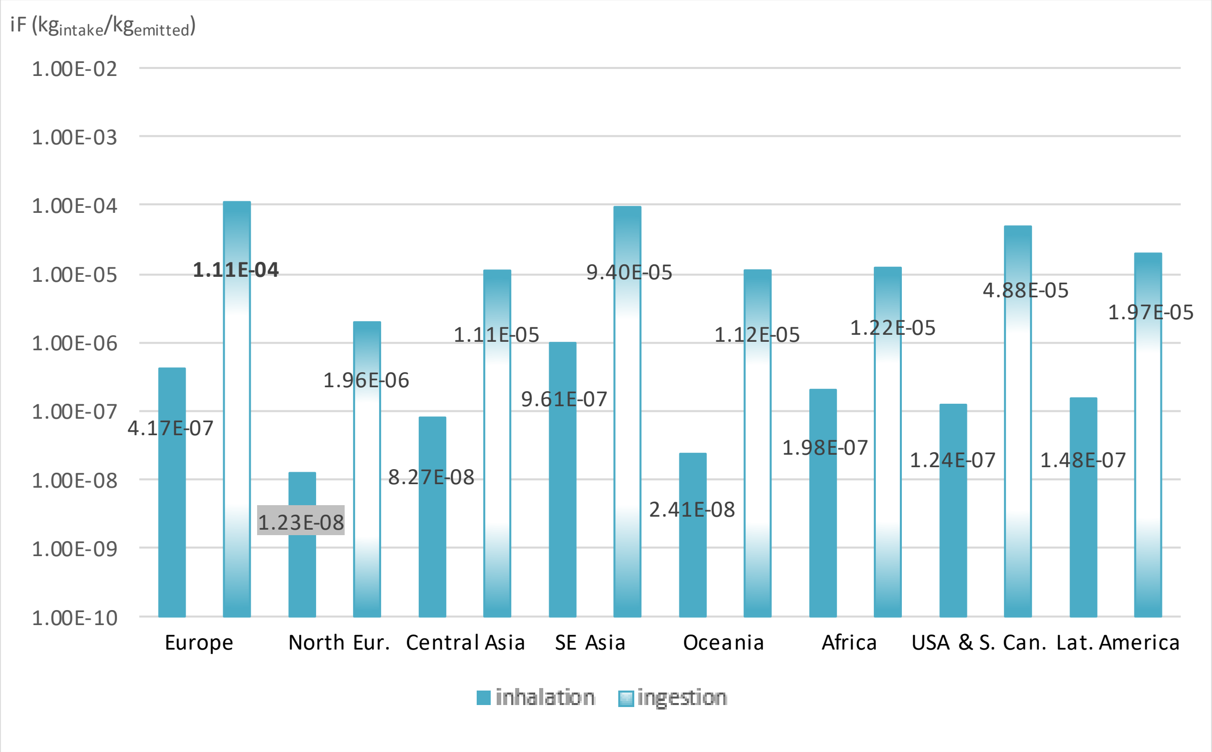

Figure 4.17. Comparison of the intake Factor of dioctyl terephthalate in different regions for inhalation and ingestion (emission into continental rural air).

Table 4.7. Intake Factor of dioctyl terephthalate in USEtox default region for inhalation and ingestion (emission into continental rural air).

Substance	**Intake Factor** **Zone**	Inhalation	Ingestion
Dioctyl terephthalate	USEtox default region	**5.66E-07**	**7.50E-05**

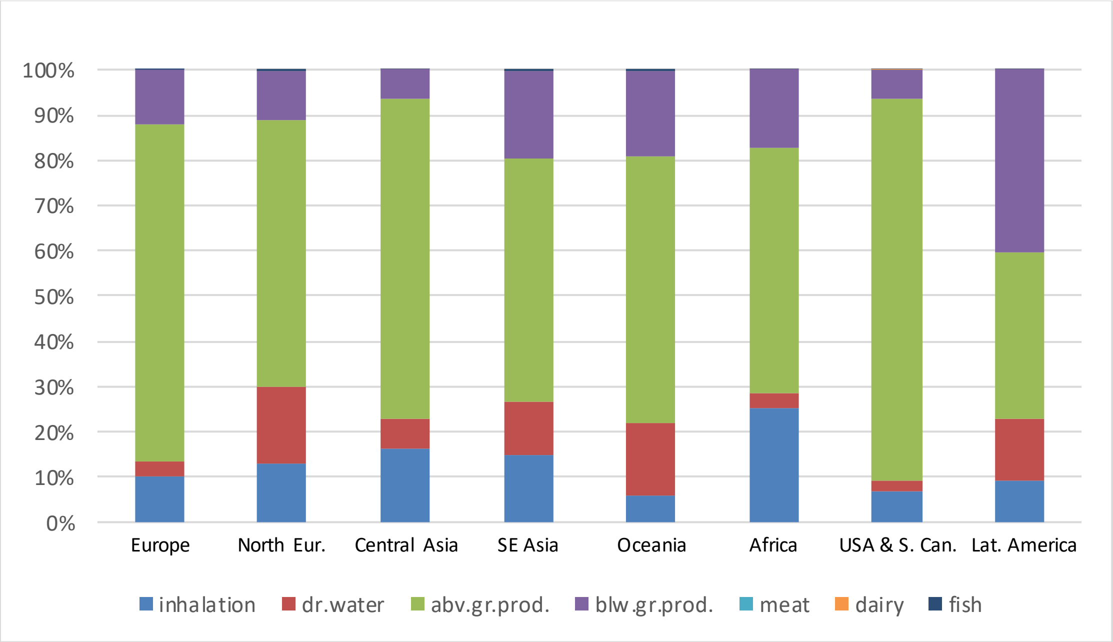

Figure 4.18. Formaldehyde intake pathway distribution in different locations (emission into continental rural air).

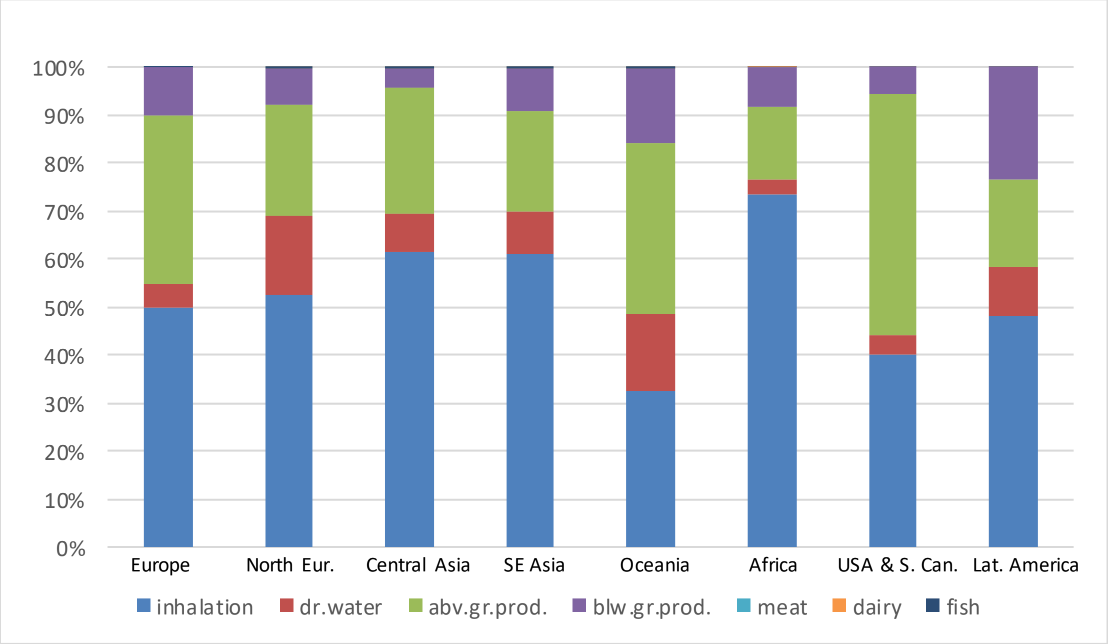

Figure 4.19. Allyl alcohol intake pathway distribution in different locations (emission into continental rural air).

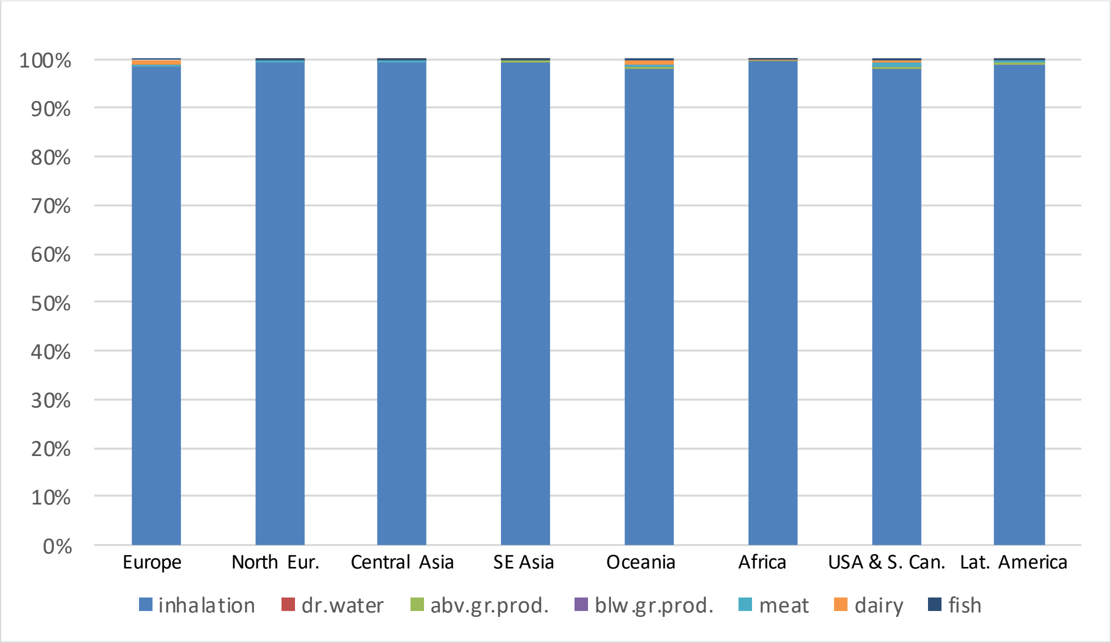

Figure 4.20. Octane intake pathway distribution in different locations (emission into continental rural air).

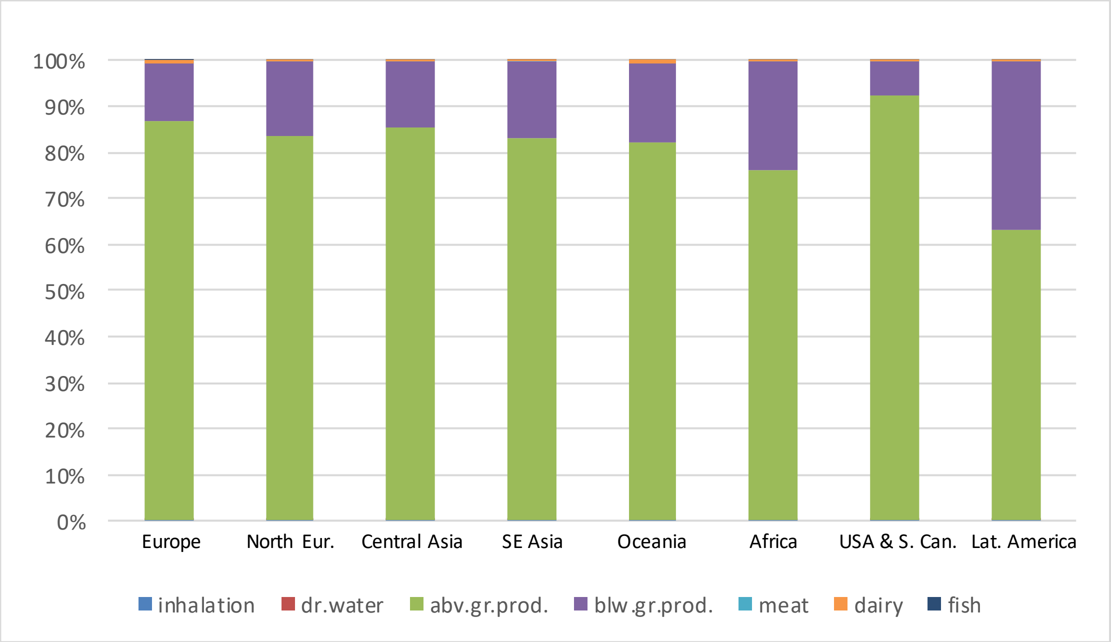

Figure 4.21. Lead intake pathway distribution in different locations (emission into continental rural air).

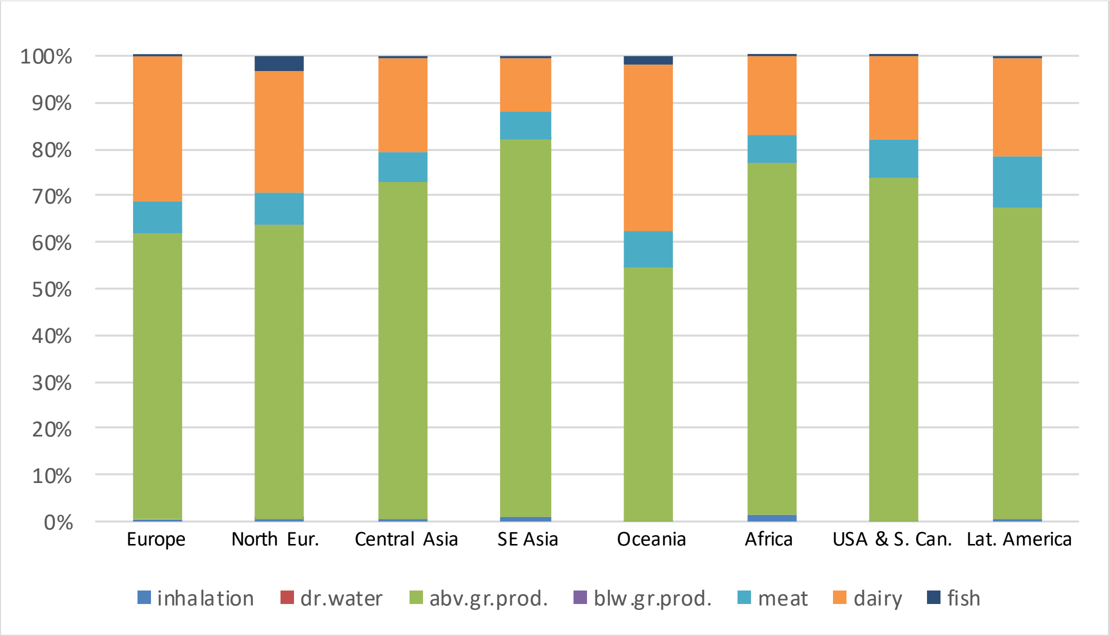

Figure 4.22. Dioctyl terephthalate intake pathway distribution in different locations (emission into continental rural air).

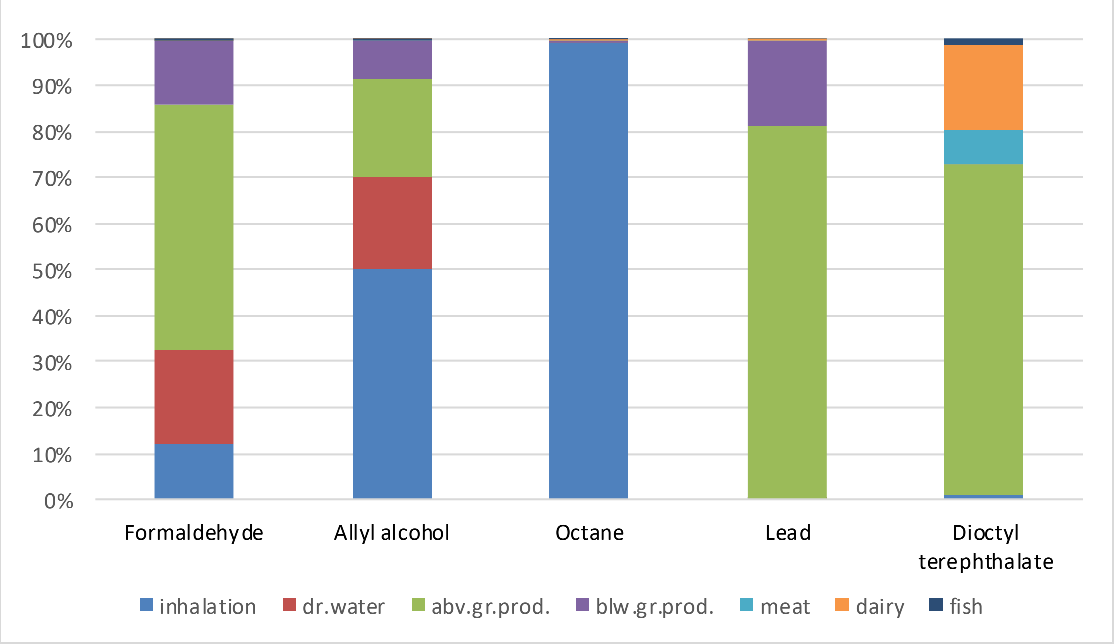

Figure 4.23. Intake pathway distribution of all substances in USEtox default region (emission into continental rural air).

Analyzing the results for an emission in the natural soil, initially comparing with the iF resulting from an emission to the rural air. Figure 4.24 shows that the iF values of inhalation of formaldehyde decreased by approximately one order of magnitude for an emission in natural soil, as this substance will be less exposed by the inhalation route. The ingestion iF of this substance also present variations of at most one order of magnitude, which will be discussed in detail. Figure 4.25 presents that allyl alcohol exhibits a behaviour similar to formaldehyde, although iF variations are less pronounced. Octane, in turn, maintains the iF values, regardless of whether the emission is released in rural air or in natural soil, as shown in Figure 4.26. This is due to the physical-chemical characteristics of this substance. Lead decreases is iF intake by approximately four orders of magnitude (Northern Europe region and Northern Canada) when the emission is released in natural soil. This reflects the persistence of lead in this compartment and the reduced migration rate when released into this compartment, resulting in reduced exposure and therefore a lower iF. Once the emission is made in natural soil, in the case of lead, its dispersion to the air will be almost zero, being the route of inhalation of this substance negligible. On the other hand, the migration rate to other compartments such as freshwater/seawater is possible, as observed in Figure 4.32 showing the intake pathway distribution. Finally, dioctyl terephthalate presents lower iF values of an order of magnitude, when it comes to an emission to natural soil because, as lead, for natural soil the results originate a lower exposure to the population for this substance, as presented in Figure 4.28.

Comparing the iF values for the emission of a substance in different regions, such as in an emission for rural air, it is concluded that the site-specific parameters of each selected region pose an important role in the calculation of the iF of a given substance. This is justified by the fact that there are iF variations of several orders of magnitude when comparing several regions.

As in the case of an emission for rural air, the iF values presented for the USEtox default region, from Table 4.8 to Table 4.12, correspond to intermediate iF values of the selected regions, both in the inhalation and intake routes.

It is observed that the most likely routes of substance intake vary substantially, depending on the emission compartment, in this case or rural air or natural soil.

First, in Figure 4.29 it can be observed that formaldehyde continues to present higher iF values for the intake route than the inhalation route. However, for an emission to the natural soil, the main route of ingestion of this substance, in addition to above-ground production, is water intake as well, presenting significant values for some regions. This result is due to the fact that formaldehyde has a high rate of migration from natural soil to aquatic compartments, thus resulting in a higher FF in this compartment, which will contribute to a higher value of iF. In regions such as Latin America, Oceania and Southeast Asia, the water intake route constitutes almost the entire iF of ingestion of this substance. As mentioned in previous cases, the high precipitation rate in these regions favors the migration of formaldehyde to aquatic compartments, therefore a higher probability of intake through drinking water. The highest iF value is observed for an emission in Southeast Asia (much higher when compared to an emission in Northern Europe, for example) mainly due to population values.

Allyl alcohol has similar intake routes, regardless of the emission region, as shown in Figure 4.30. The main intake route of this substance is water intake for all regions although in Northern Europe and the African continent the fraction of inhalation iF is also visible. Although not a very significant result, once again the reduced precipitation rate in these areas favors the deposition of allyl alcohol in the air rather than depositing in aquatic compartments. As in the case of a formaldehyde emission, the highest iF value is showed for the Southeast Asia region.

Figure 4.31 shows that, as in the case of an emission into the rural air, octane has a uniform behaviour, despite the emission region, as the most likely intake route is undoubtedly the inhalation route, due to the physical-chemical characteristics of this substance. It should also be noted that although the inhalation route is dominant in this substance, the emission region also poses an important role in the amount that is actually intaked from this pollutant, since there are discrepancies in the values of iF (e.g. the inhalation iF corresponding to an emission in Southeast Asia is 2.52E-06 kg intake/kg emitted, while for an emission in Northern Europe is 8.55E-08 kg intake/kg emitted), due to population values.

Lead presents the main intake route in almost all regions for the above-ground production exposure. However, in Latin America is observed a high intake fraction of this substance related to below-ground production, due to the fact that this region has higher consumption of products from below-ground production, in relation to above-ground production (Figure 4.32). In the Northern European and Oceania regions, the main route of lead intake is clearly through the consumption of fish. This is mainly due to differences in consumption patterns in each region and also the inherent chemical characteristics of lead. This is a substance that when emitted into the soil tends to deposit there, although there are fractions that migrate to aquatic compartments. Lead is a substance with a very large bioaccumulation factor in fish, greater than a unit, indicating that the concentration in this organism is greater than of the medium from which this substance was released. Being Northern Europe and Oceania two regions with a much higher fish consumption than the rest, this will result in a high iF value for this intake route. Depending on the emission region, the iF values of lead intake show large discrepancies, indicating large variations in the amount that is actually consumed of this substance. For instance, an emission into natural soil in the Southeast Asian region presents a value of iF higher than three orders of magnitude, when compared to an emission in the Northern Europe region, mainly due to population values.

Finally, dioctyl terephthalate presents above-ground production as the main intake route, observed in Figure 4.33, but as in the case of an emission to rural air in the Oceania region, dairy products consumption constitutes an important fraction of the total value of the iF of intake of this substance. As in the case of substance emissions presented earlier, the emission region strongly influences the amount that is actually consumed of dioctyl terephthalate when an emission occurs in natural soil. For example, the iF associated with this emission in Southeast Asia is almost two orders of magnitude greater than the iF associated with an emission in Northern Europe.

Analyzing the results of Figure 4.34, corresponding to the intake pathway distribution of all substances in USEtox default region, these present values common to most regions presented in the previous graphs. It should be noted that formaldehyde in this region exhibits a similar behaviour to the region of Central Asia, Southeast Asia and Oceania, where the main route of ingestion of this substance is by drinking water. And dioctyl terephthalate has a considerable iF in the fish intake route, because the USEtox default region is modeled, with a high fish consumption per capita, compared to other regions.

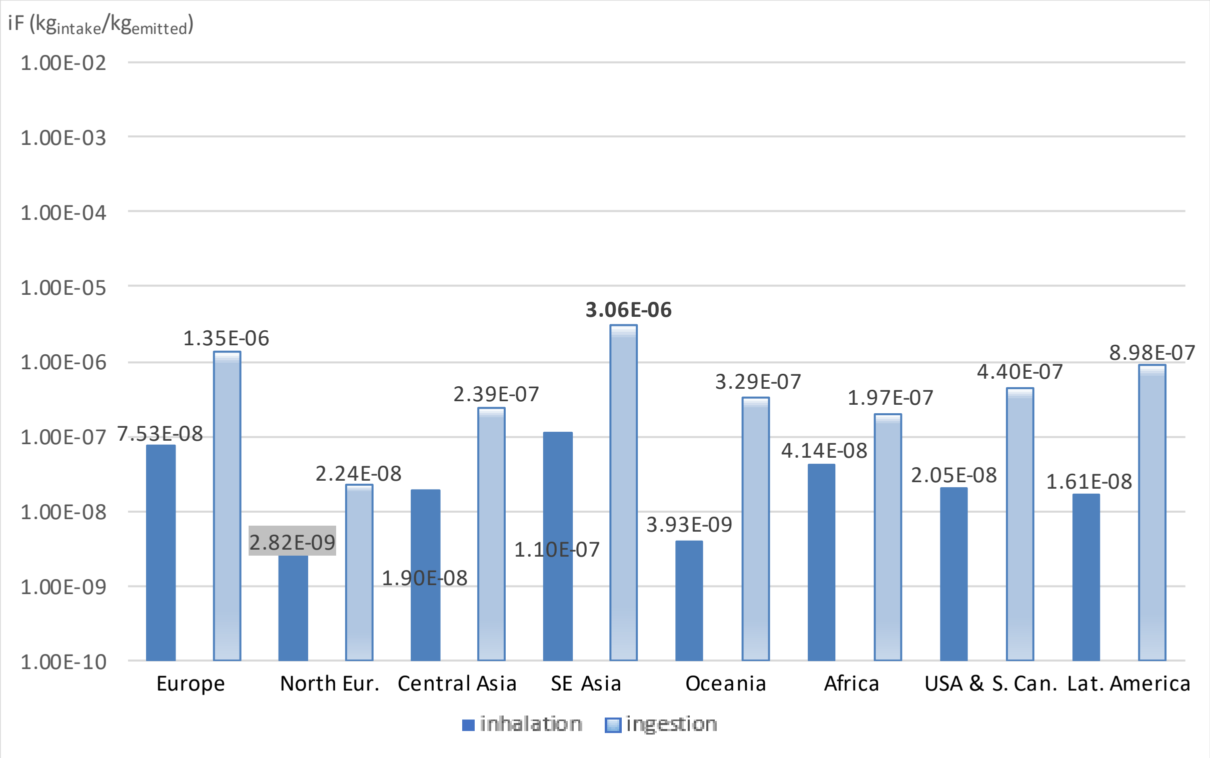

Figure 4.24. Comparison of the intake Factor of formaldehyde in different regions for inhalation and ingestion (emission into continental natural soil).

Table 4.8. Intake Factor of formaldehyde in USEtox default region for inhalation and ingestion (emission into continental natural soil).

Substance	**Intake Factor** **Zone**	Inhalation	Ingestion
Formaldehyde	USEtox default region	**9.87E-08**	**4.85E-06**

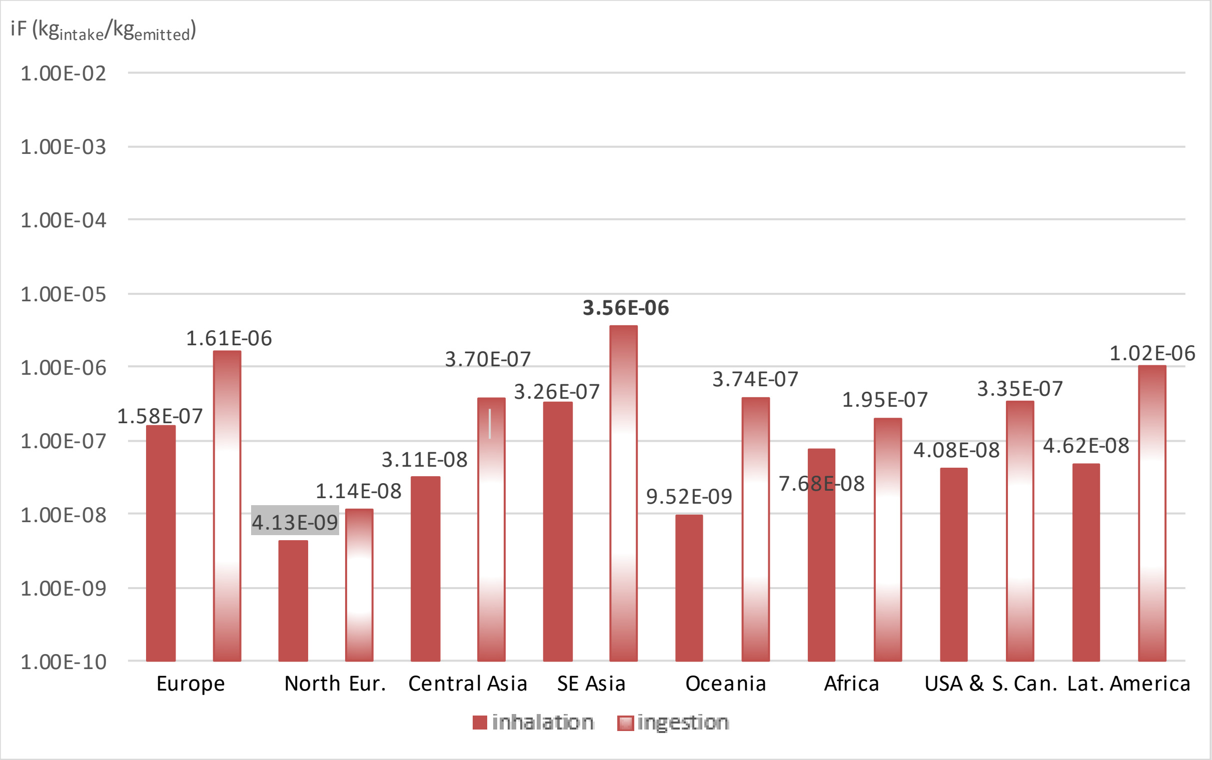

Figure 4.25. Comparison of the intake Factor of allyl alcohol in different regions for inhalation and ingestion (emission into continental natural soil).

Table 4.9. Intake Factor of allyl alcohol in USEtox default region for inhalation and ingestion (emission into continental natural soil).

Substance	**Intake Factor** **Zone**	Inhalation	Ingestion
Allyl alcohol	USEtox default region	**2.32E-07**	**6.61E-06**

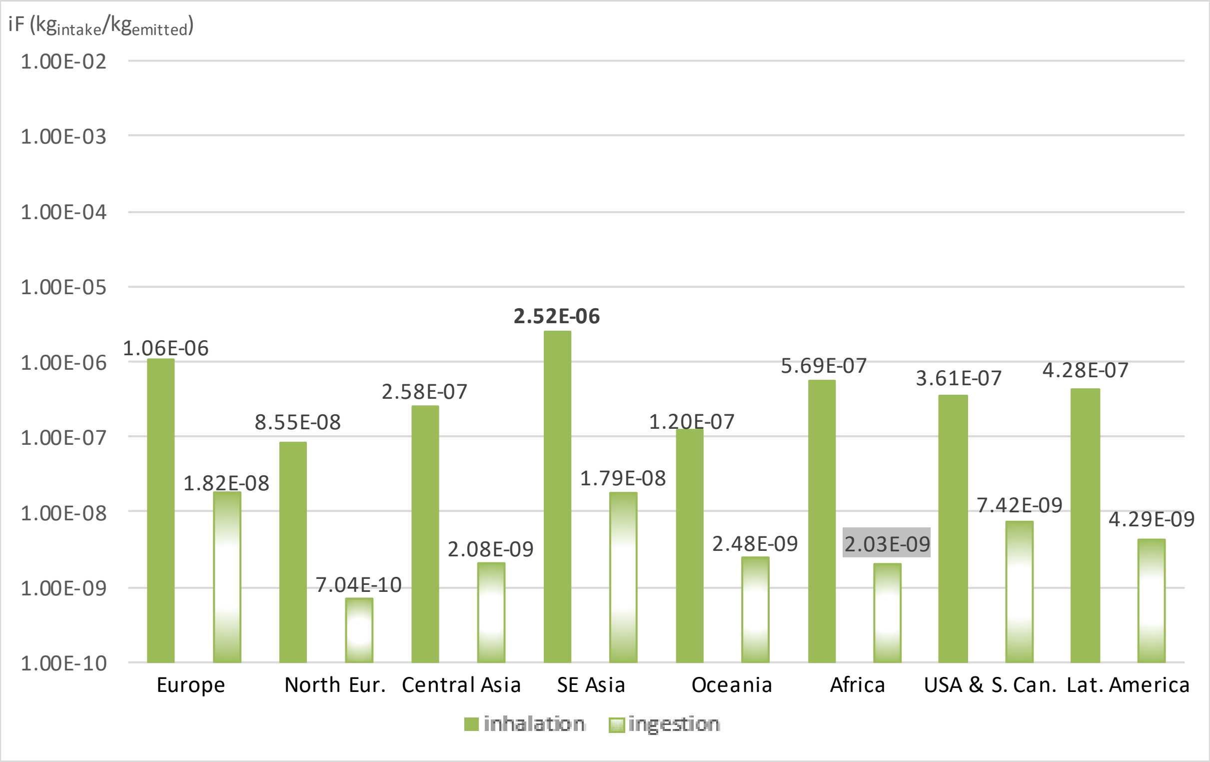

Figure 4.26. Comparison of the intake Factor of octane in different regions for inhalation and ingestion (emission into continental natural soil).

Table 4.10. Intake Factor of octane in USEtox default region for inhalation and ingestion (emission into continental natural soil).

Substance	**Intake Factor** **Zone**	Inhalation	Ingestion
Octane	USEtox default region	**1.42E-06**	**1.34E-08**

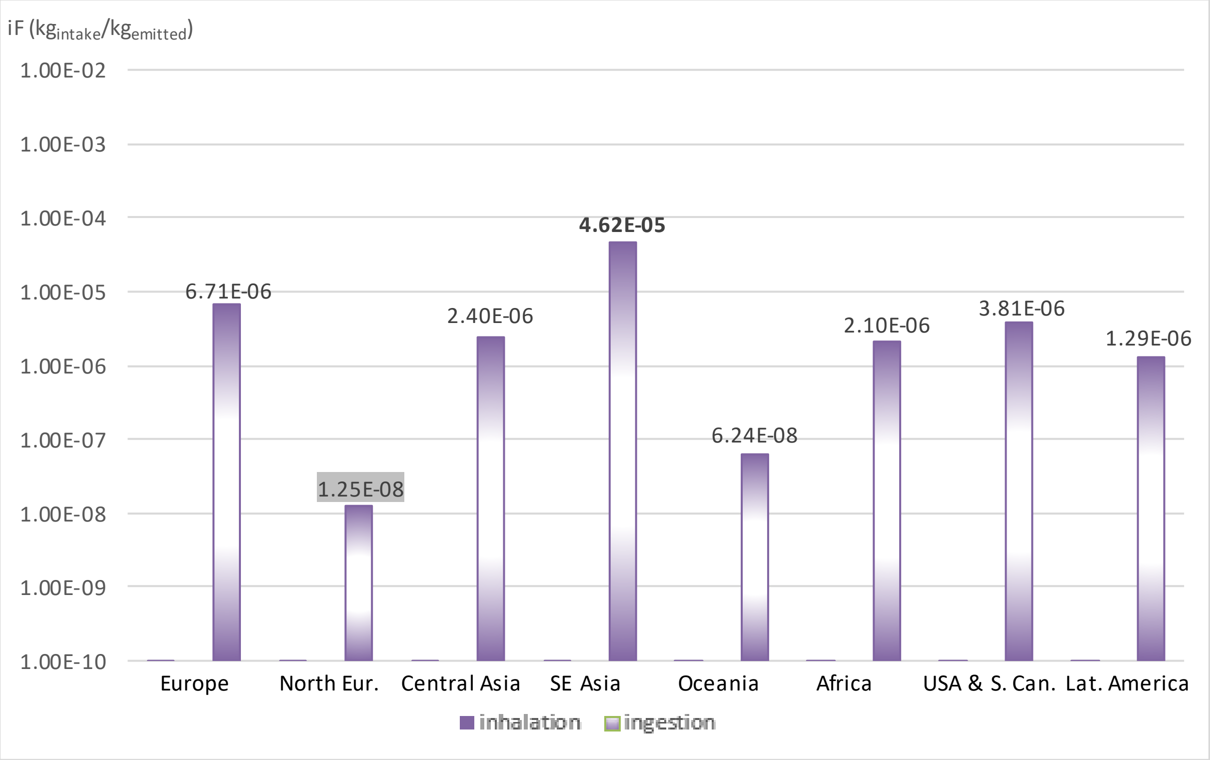

Figure 4.27. Comparison of the intake Factor of lead in different regions for inhalation and ingestion (emission into continental natural soil).

Table 4.11. Intake Factor of lead in USEtox default region for inhalation and ingestion (emission into continental natural soil).

Substance	**Intake Factor** **Zone**	Inhalation	Ingestion
Lead	USEtox default region	**3.09E-25**	**3.45E-06**

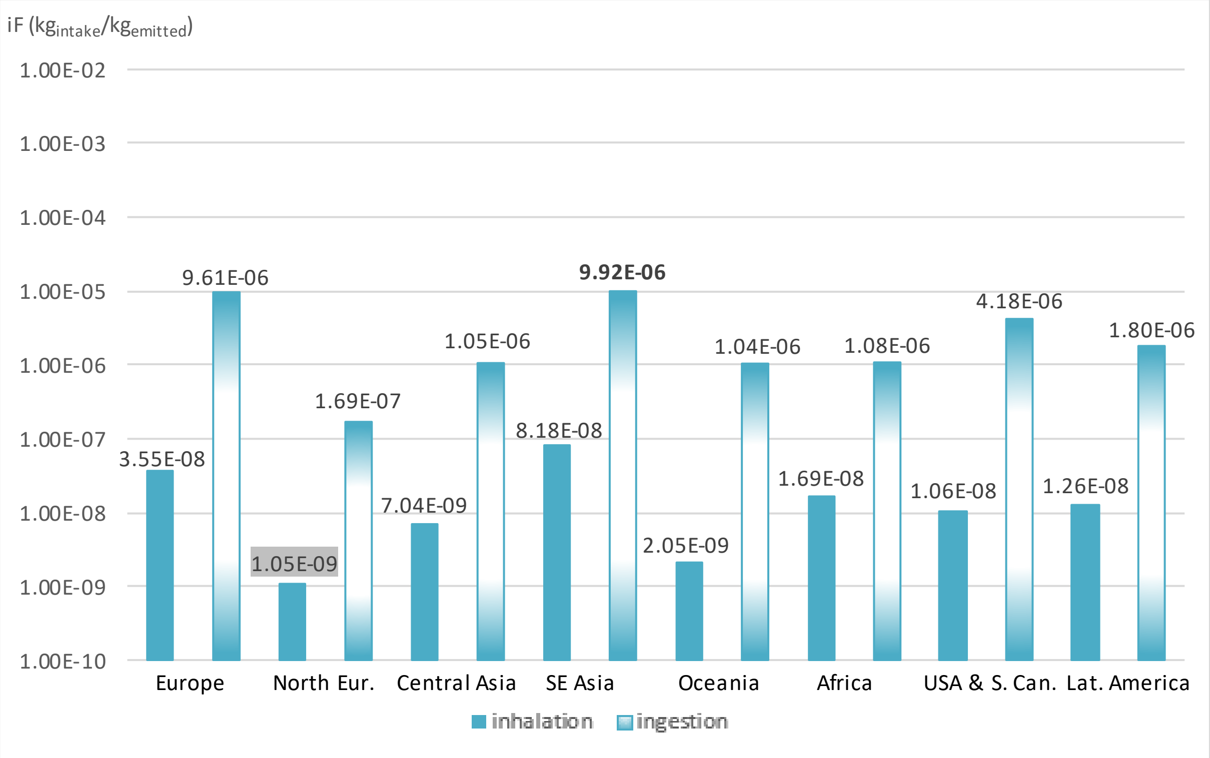

Figure 4.28. Comparison of the intake Factor of dioctyl terephthalate in different regions for inhalation and ingestion (emission into continental natural soil).

Table 4.12. Intake Factor of dioctyl terephthalate in USEtox default region for inhalation and ingestion (emission into continental natural soil).

Substance	**Intake Factor** **Zone**	Inhalation	Ingestion
Dioctyl terephthalate	USEtox default region	**4.81E-08**	**8.85E-06**

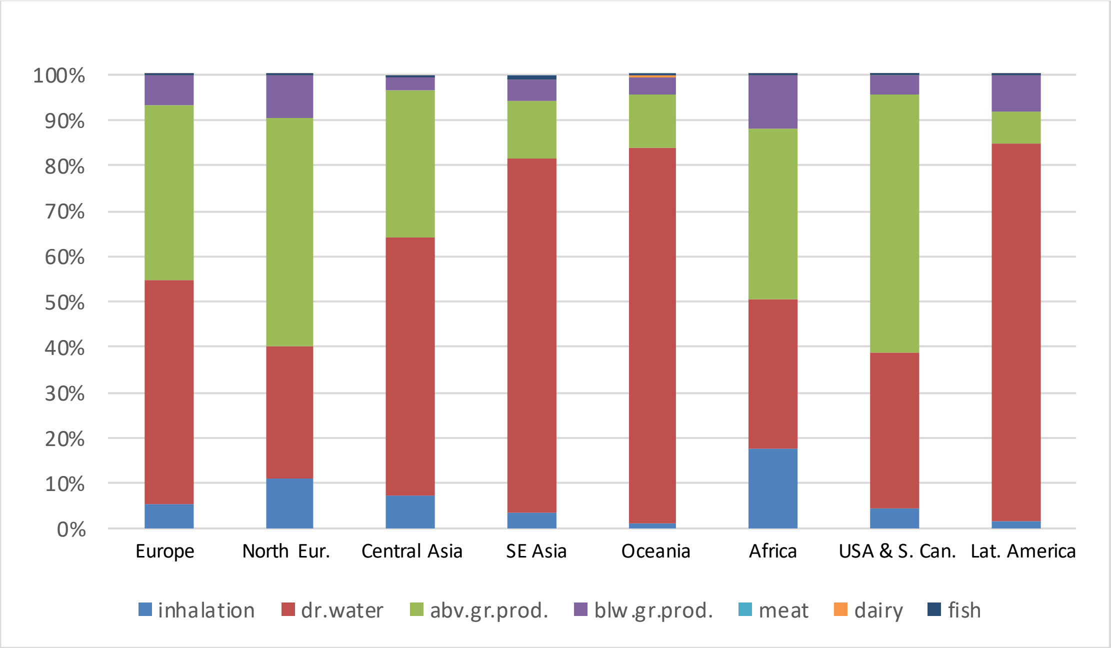

Figure 4.29. Formaldehyde intake pathway distribution in different locations (emission into continental natural soil).

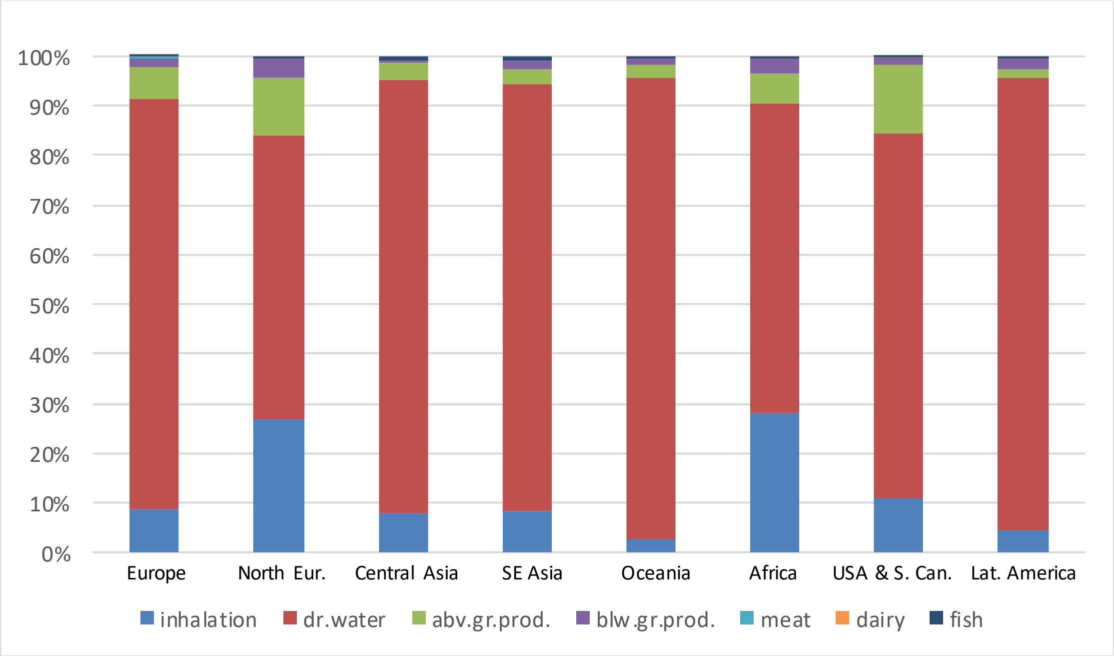

Figure 4.30. Allyl alcohol intake pathway distribution in different locations (emission into continental natural soil).

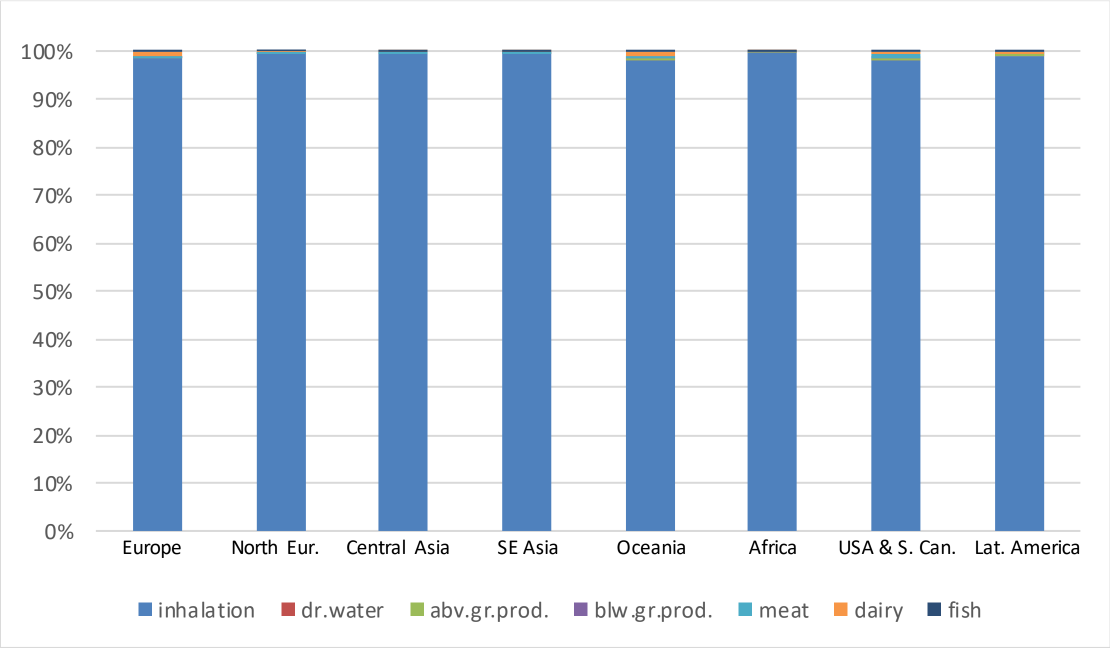

Figure 4.31. Octane intake pathway distribution in different locations (emission into continental natural soil).

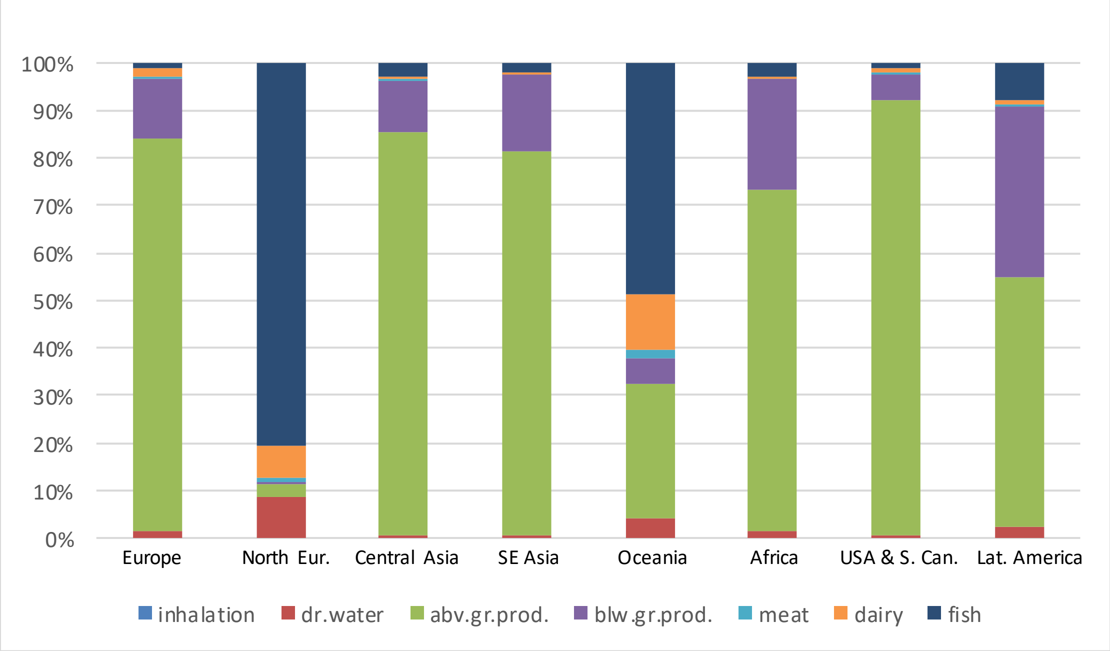

Figure 4.32. Lead intake pathway distribution in different locations (emission into continental natural soil).

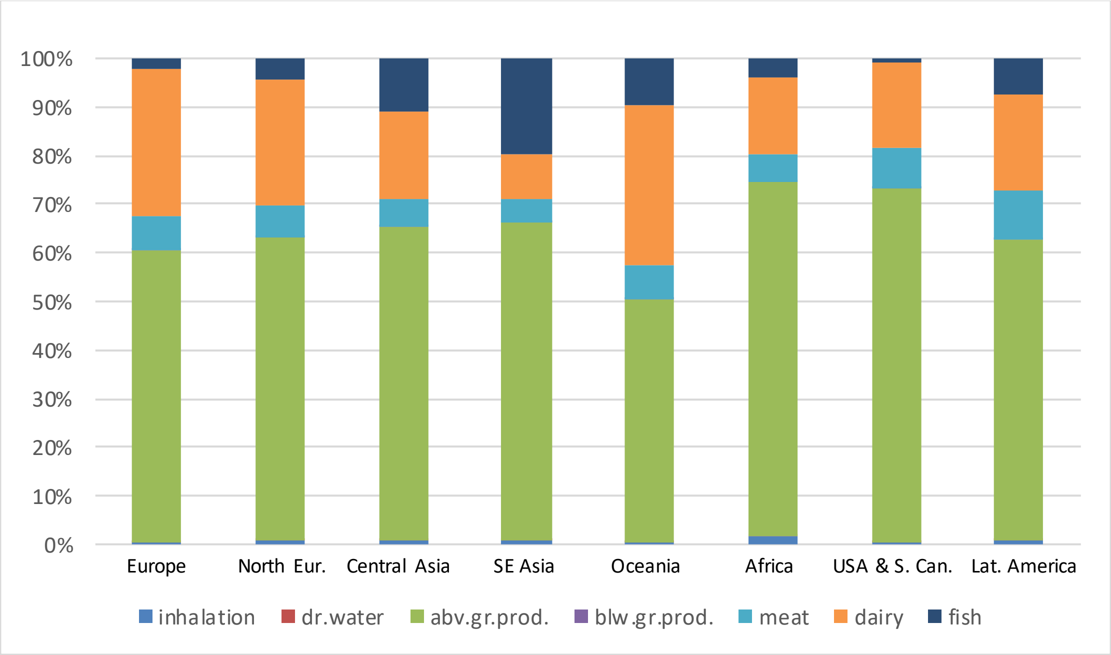

Figure 4.33. Dioctyl terephthalate intake pathway distribution in different locations (emission into continental natural soil).

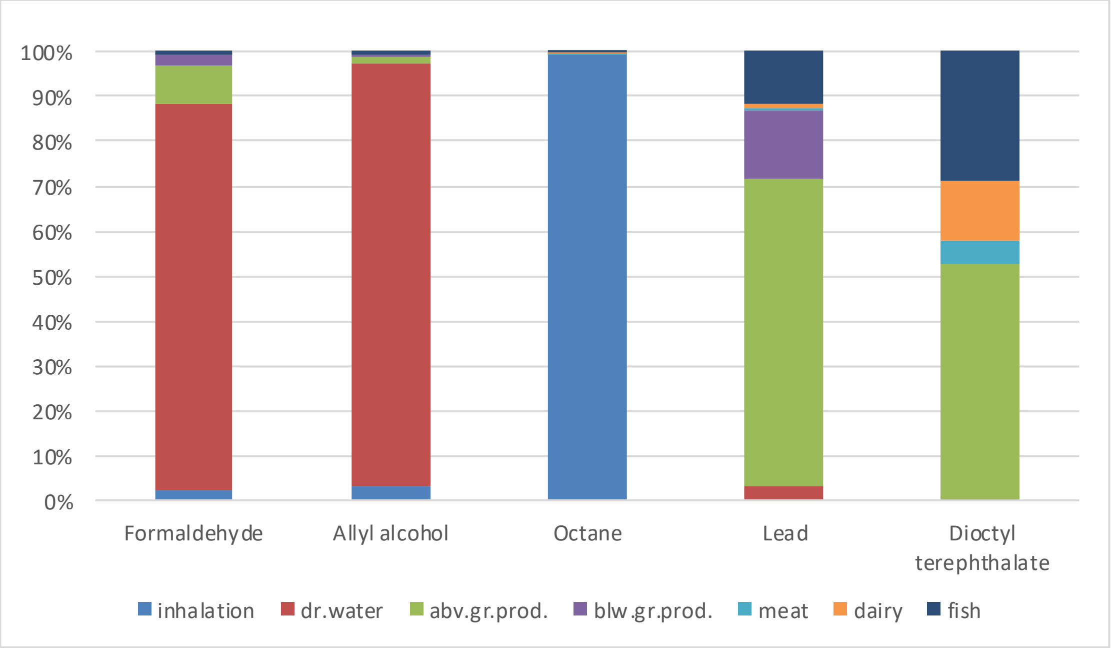

Figure 4.34. Intake pathway distribution of all substances in USEtox default region (emission continental natural air).

4.1.3. Effect factors

As mentioned before in this thesis, the effect factor (EF) is not dependent of the site-specific conditions, since it is related only to the effect (toxicity) of the substance in humans.

Thus, the effect factors have the same value for all regions and then this analysis was made only for the default region. Table 4.13 presents the effect factors for ingestion and inhalation, counting carcinogenic and non-carcinogenic effects.

From this table it can be observed which are the substances with the highest toxic potential, taking into account the route of exposure and inhalation and which have carcinogenic effects or not. It is important to note that there are no data on the toxicity of some substances and, therefore, these ones are not shown in the table. The lack of results does not mean that the substances are not toxic, these values may be due to insufficient data about their potential toxicity.

For inhalation effect and carcinogenic, is showed that formaldehyde is a substance more harmful than lead, since it presents an $EF_{inh,canc}$ two orders of magnitude higher. From this result, it can be concluded that when intaked the same amount of these two substances, more cases of carcinogenic effects will be verified when formaldehyde is intaked. The remaining three substances do not present data on their toxicity, so no conclusions can be made about their toxicity potential. As mentioned earlier, the lack of results does not mean that the substances are not toxic and, therefore, uncertainty in its toxicity should be considered.

Then, analyzing the EFs for an inhalation route, but with non-cancer effects, only the octane does not present data on its toxicity. Of the remaining substances, the most hazardous is lead, since it presents an $EF_{inh,non\text{-}canc}$ higher in more than two orders of magnitude to that of the remaining substances. From these results it is inferred that lead dominates the toxicological impacts in case of non-cancer effects, in this intake route.

Finally, by analyzing the results of the EF, but for the ingestion route, they are also divided into carcinogenic and non-carcinogenic effects. In the case of carcinogenic effects, the highest value of $EF_{ing,canc}$ is presented by lead, although reduced (with equal value to that presented for the inhalation route). Formaldehyde, in this case, has an $EF_{ing,canc}$ lower than that of lead (approximately one order of magnitude), and the null value for allyl alcohol indicates that this substance has no carcinogenic effects. As for non-carcinogenic effects, the results presented are the same as for the inhalation route, that is, lead dominates the toxicological impacts in case of non-cancer effects, regardless of the intake route.

These results are due to the toxicological characteristics of the substances, namely the ED50, which quantifies a human-equivalent lifetime dose per person that causes a cancer/non-cancer disease probability of 50% after inhalation/ingestion. Therefore, the lower this value, the more harmful the substance will be in the corresponding intake route. The value shown for $EF_{inh,canc}$ of formaldehyde is due to the fact that this substance has an $ED50_{inh,canc}$ much lower than that of lead. In the case of a lead emission, for the $EF_{non\text{-}canc}$ on both ingestion routes, this high value is justified by a very low value of $ED50_{inh,non\text{-}canc}$ and $ED50_{ing,non\text{-}canc}$ compared to that of the other substances.

Table 4.13. Effect Factors of the substances selected for inhalation and ingestion routes (including cancer and non-cancer effects.

Substance	Inhalation		Ingestion	
	cancer	non-canc.	Cancer	non-canc.
Formaldehyde	**1.06E+00**	**8.47E-03**	**2.05E-03**	**8.47E-03**
Allyl alcohol	**-**	**5.29E-02**	**0.00E+00**	**5.29E-02**
Octane	**-**	**-**	**-**	**-**
Lead	**2.46E-02**	**8.63E+00**	**2.46E-02**	**8.63E+00**
Dioctyl terephthalate	**-**	**1.00E-04**	**-**	**1.00E-04**

4.2. Sensitivity analysis to site-specific parameters of the USEtox model

The toxicological assessment carried out for the regions in the USEtox model showed that the site-specific parameters present some influence in the results for the same substances. This chapter aims to understand the sensibility that some site-specific parameters can have on the calculation of characterization factors of substances using the USEtox model. The parameters analyzed are selected based on the influence observed in the assessment of the results. Then, this chapter will be described by varying the relevant site-specific parameters in the calculation of FF and iF, obtained in the analysis of the previous results. For the analysis of sensitivity of the FF results to site-specific parameters, the following site-specific parameters will be varied: land area, sea area and precipitation rate, both on a continental scale. For analysis to the iF will be varied the human population and parameters referring to production-based intake-rates, in this case above-ground produce and fish ingestion, also on a continental scale. It should be mentioned that the parameters considered constant for all regions of the USEtox (e.g. soil erosion, human breathing rate and water ingestion), were not varied in this analysis.

Based on this parameters, three scenarios were developed for each parameter selected, varying one, two or three orders of magnitude from the result presented for the USEtox default region, depending on the parameter under analysis. In the case of the land area parameters and the ones for population and production-based intake rates (above-ground produce and fish ingestion), the three defined scenarios are the following: the default, which assumes a value equal to that defined for the USEtox default region; scenario 1, where the value of this parameter is reduced by two orders of magnitude and scenario 2, where it is increased by two orders of magnitude. This variation of orders of magnitude was selected in order to overcome the typical variation of them, between the different regions, and conclude how a variation of these parameters, with a magnitude greater than the average, influences the results. For the rain rate, the scenarios adopted were the default; scenario 1, where the value of this parameter is reduced in an order of magnitude and scenario 2, where it is increased in an order of magnitude. This was the variation selected for the different scenarios of this parameter because it was the maximum allowed by USEtox. Finally, for the sea area parameter, scenario 1, presents a value three orders of magnitude lower than the one presented for the default scenario, and scenario 2 presents one three orders of magnitude higher. This magnitude of variation was selected to understand how the behaviour of substances that tend to deposit in aquatic compartments is influenced if the sea area is abruptly increased or reduced. These scenarios are compared with the default region of the USEtox model, which presents average values for the site-specific parameters. Emissions for rural and natural soil are also considered.

Figure 4.35 shows the influence on the calculation of the fate factor associated with the variation of land area. The land area parameter was previously identified as being potentially influential in FF when it comes to a lead emission. Because this is a substance that is mainly deposited in the soil, the value of this parameter becomes even more important. As can be concluded from the figure, the larger the land area, the higher the FF value of lead, especially in the natural soil. Although the default FF value does not have a significant difference from scenario 2, when compared to scenario 1, this difference is more than one order of magnitude. Suggesting that for regions with very small land areas, the FF value of lead in soil compartments decreases substantially because it will tend to deposit in other compartments as sea water or fresh water, where the persistence of this substance is lower.

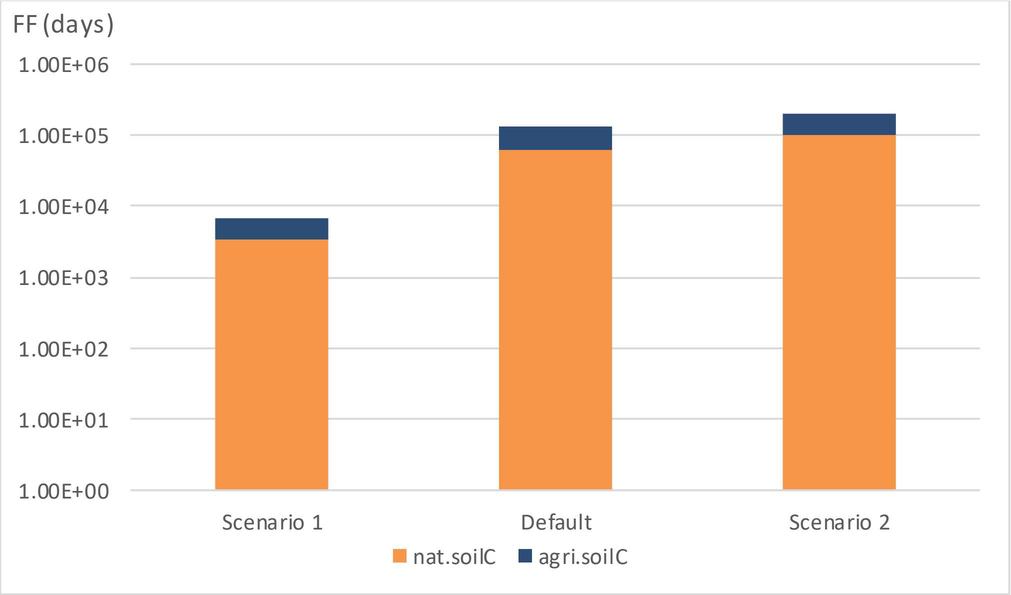

Figure 4.35. Influence on the Fate Factor of lead with variation of the land area parameter - Emission into continental rural air.

Figure 4.36 shows the influence on the calculation of the fate factor associated with the variation of rain rate. Using the same emission from the previous example, unlike the previous case, and as can be concluded from the results of the figure, the higher the rain rate, the lower the FF value of the lead, mainly in the natural soil. This is because the degradation of this substance in the soil will be greater and therefore will result in less persistence. Also, the transport of lead by the action of the rain to other compartments where the persistence of this substance is lower, contributes to this result. Between scenario 1 and scenario 2, a FF difference of more than one order of magnitude is visible.

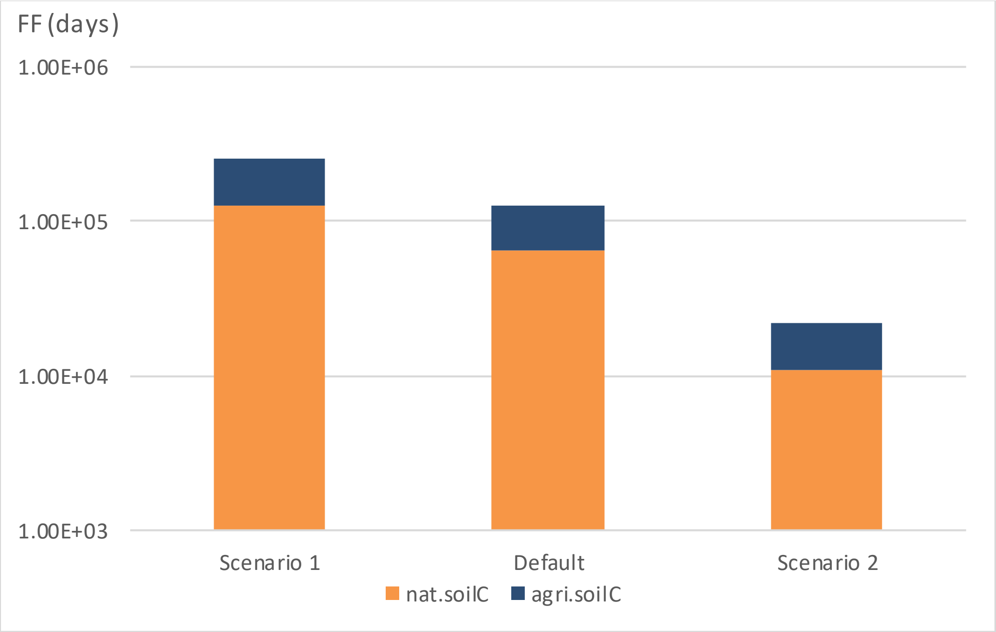

Figure 4.36. Influence on the Fate Factor of lead with variation of the rain rate parameter - Emission into continental rural air.

Figure 4.37 shows the influence on the calculation of the fate factor associated with the variation of sea area. The sea area parameter proved to be important in FF when it comes to a formaldehyde emission in rural air. Since this is one of the main deposition compartments of this substance, the value of this parameter becomes even more important. As can be concluded from the figure, the larger the sea area, the higher the FF value of formaldehyde, especially in the sea water compartment. Although the FF value does not have a significant difference between the different scenarios, when analyzing this value only in the sea water compartment, it is concluded that it increases abruptly with the increase of the sea area. This result suggests that by increasing the sea area, formaldehyde will have a more tendency to deposit in this compartment, thus reducing persistence in others in a similar proportion and, therefore, the overall difference of FF is not significant.

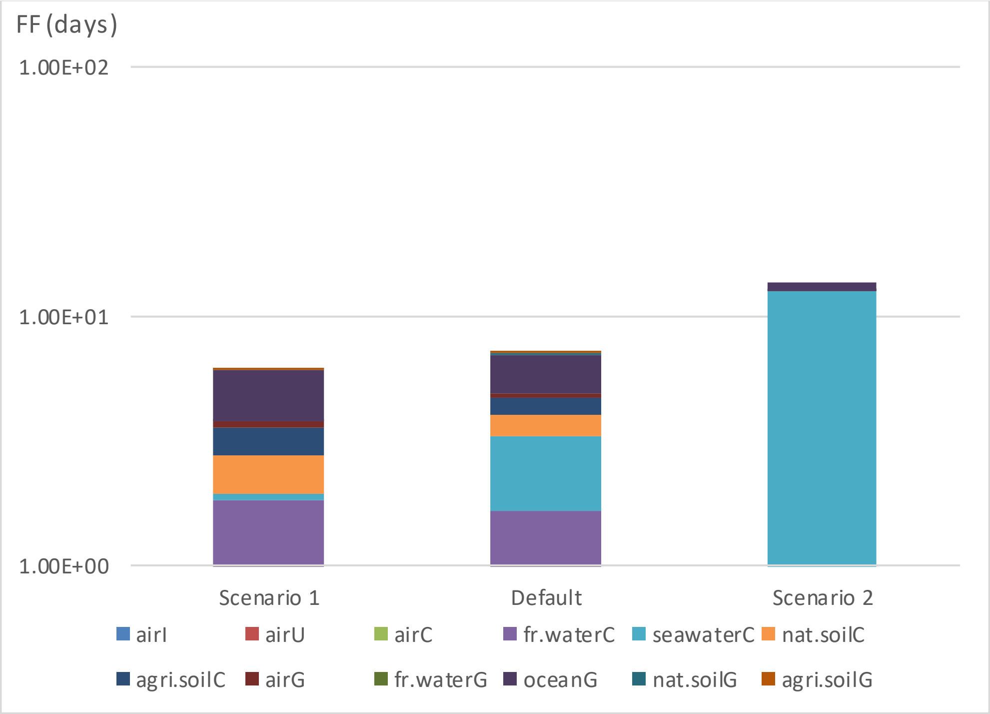

Figure 4.37. Influence on the Fate Factor of formaldehyde with variation of the sea area parameter - Emission into continental rural air.

Site-specific parameters also influence the iF value of substances, especially production-based intake rates. Figure 4.38 shows the influence on the calculation of the intake factor associated with the variation of fish consumption. Fish consumption has previously been identified as a potentially influential parameter in iF when it comes to a lead emission in natural soil. Being this a substance with a very large bioaccumulation factor in fish, greater than a unit, this indicates that the concentration in this organism is greater than that of the medium from which lead was released. Therefore, the value of fish consumption per capita is important when addressing such an emission. As can be concluded from the figure, the higher the fish consumption per capita, the higher the value of the lead iF, associated only with this intake route. Although the default iF value does not have a significant difference from scenario 1, when compared to scenario 2, this difference is more than one order of magnitude. Suggesting that for regions with a very high fish intake, the iF value of lead increases substantially on this intake route.

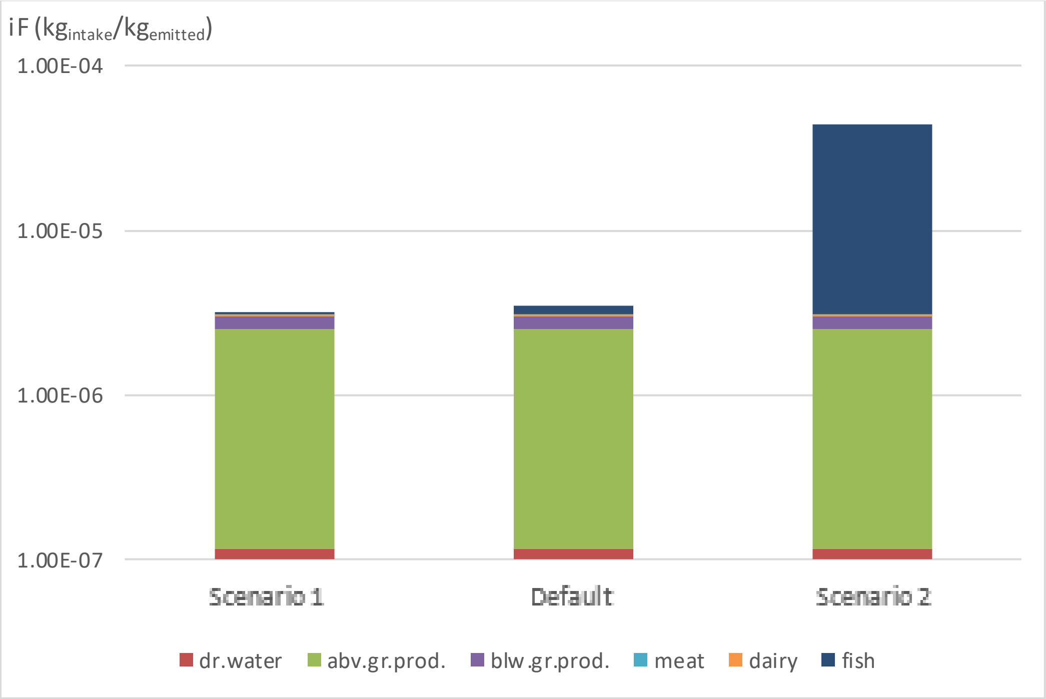

Figure 4.38. Influence on the intake Factor of lead with variation of the fish consumption parameter - Emission into continental natural soil.

Figure 4.39 shows the influence on the calculation of the intake factor associated with the variation of human population. The parameter referring to the human population, influences, on a large scale, the value of the iF of substances. This parameter was previously identified as potentially influential in iF for the emission of any substance. An emission of formaldehyde in rural air was used as an example. As can be concluded from the figure, the larger the human population of a region, the greater the iF on any route of inhalation or ingestion. The difference between different scenarios is approximately two orders of magnitude, indicating this result that the iF value grows approximately linearly, with the increase of the human population. As would be expected, increasing human exposure will result in a higher iF.

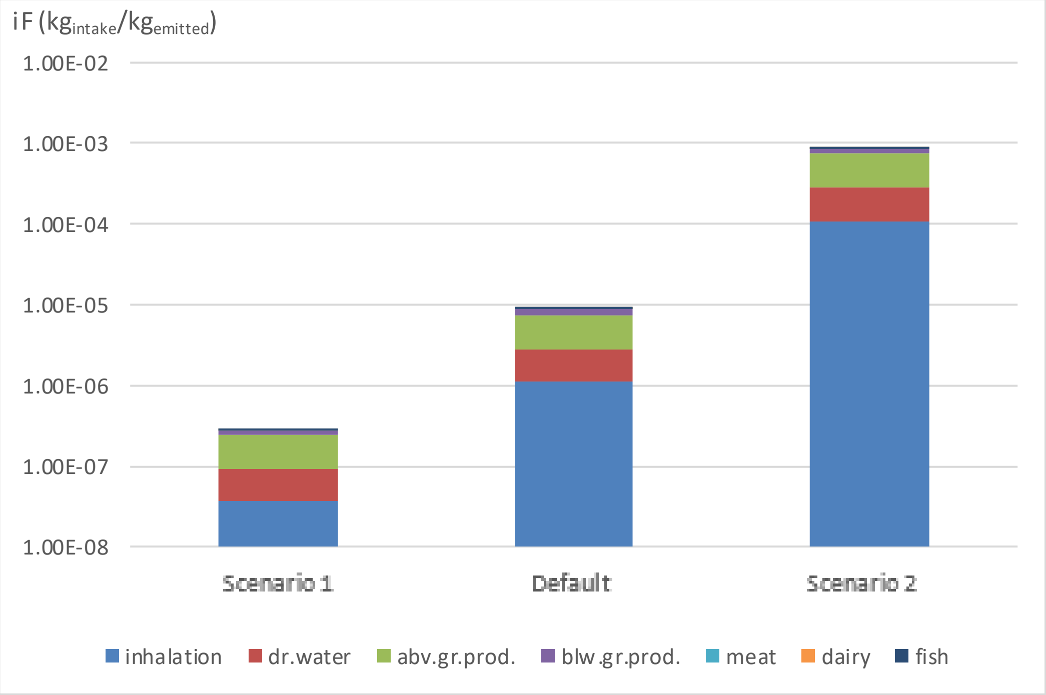

Figure 4.39. Influence on the intake Factor of formaldehyde with variation of the human population parameter - Emission into continental rural air.

Figure 4.40 shows the influence on the calculation of the intake factor associated with the variation of above-ground produce consumption, using a lead emission to rural air. Because this is a substance with high persistence in soil, this indicates that the concentration in products resulting mainly from above-ground production, will be high. Therefore, the value of the consumption of this type of products is important when addressing an emission of this type. As can be seen from the figure, the higher the consumption of products resulting from above-ground production, the higher the value of the lead iF, associated only with this intake route. The difference in iF values from scenario 1 to default is approximately one order of magnitude, and the default for scenario 2 is almost two orders of magnitude. Suggesting that for regions with very high consumption of products from above-ground produce, the value of the lead iF increases substantially on this intake route.

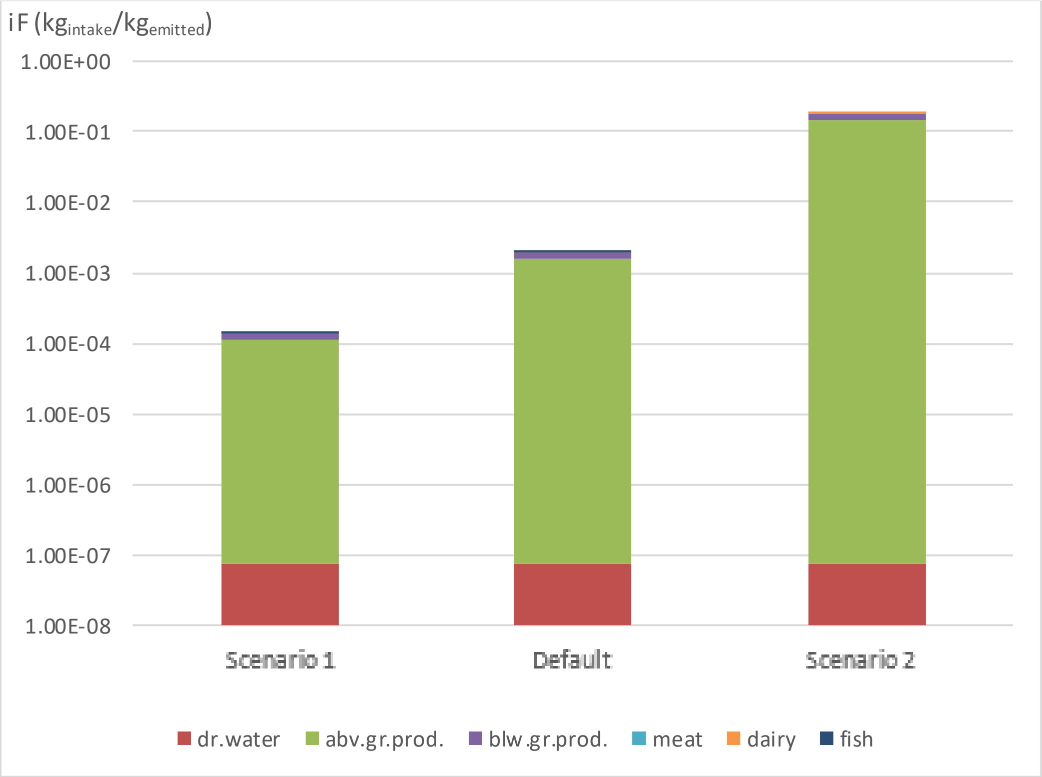

Figure 4.40. Influence on the intake Factor of lead with variation of the above-ground produce consumption parameter - Emission into continental rural air.

Figure 4.41 shows the influence on the calculation of the intake factor associated with the variation of rain rate. The rain rate parameter also influences the iF of substances. Since this is a parameter that increases exposure in aquatic compartments, its analysis is important, especially in intake routes associated with water intake. Being formaldehyde a substance with considerable persistence in aquatic compartments, this was the substance used in this analysis. As can be concluded from the figure, the higher the rain rate, the higher the value of the formaldehyde iF, associated only with the intake water ingestion route. Although the total iF value between different scenarios has no significant differences, when comparing scenario 2 and scenario 1 the iF associated with water drinking is higher in an order of magnitude. Suggesting that for regions with very high rain rates, exposure in aquatic compartments will be higher.

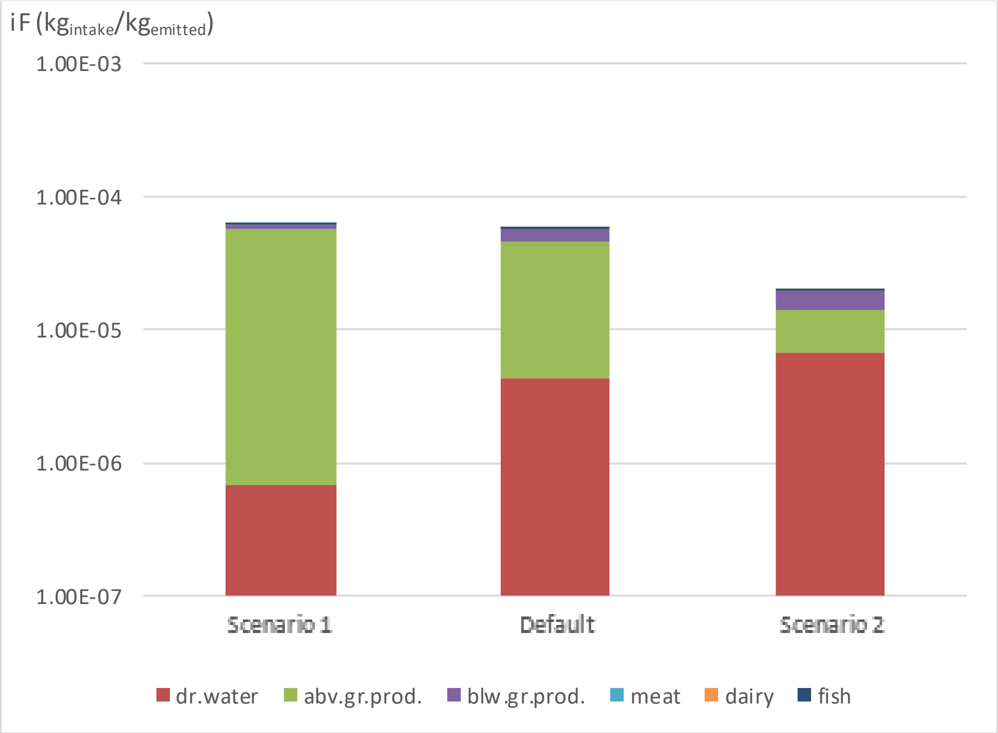

Figure 4.41. Influence on the intake Factor of formaldehyde with variation of the rain rate parameter - Emission into continental natural soil.

5. CONCLUSIONS

5.1. Main conclusions of the work

The objectives of this thesis were to analyze and compare the characterization factors associated with chemical substances emissions in different regions of the world; further understanding how the site-specific parameters characteristic of each region are obtained and inherent limitations of their definition, and perform a sensitivity analysis to the parameters identified as promising, for the results obtained for the fate factor and intake factor for the different substances, in the regions analyzed, in an attempt to understand whether this analysis is, or not, sensitive to the variation of site-specific parameters. In this thesis an insight about the main objective, associated with the life-cycle environmental impacts of substances emission was provided. Those insight were the use of a model that addresses the site-specific characteristics of the substance emission site, in order to understand the influence that those can have on the characterization factors of these substances. To achieve this objective the USEtox model was used, a consensus model developed under the UNEP-SETAC Life Cycle Initiative that provides characterization factors for human toxicological and freshwater ecotoxicological impacts of chemical emissions.

The present thesis was carried out to demonstrate the importance of environmental site-specific parameters on the value of the characterization factor associated with chemical substance emissions. These characteristics influence the factors used to quantify the environmental impacts, using the USEtox method. The site-specific parameters influence the fate factor and intake factor of the substance. The first depends only on the site-specific parameters of the site and emission compartment, in this case on a continental scale. They also influence the intake factor, since it is also dependent on parameters such as population and, mainly, production-based intake rates, also on a continental scale. Effect factors are only influenced by the characteristics of the substances because they are not dependent of the site-specific conditions since it is related only to the effect (toxicity) of the substance in humans.

The use of regions in USEtox did not present large variations in FF and iF, only a few exceptions. These cases correspond to the different persistence of lead presented in some regions, as well as the different iF values presented for all substances. For example, considering an emission of lead to rural air, the FF value is larger on the African continent when compared to Latin America. This result is due to the site-specific parameters of the emission site: the fact that the African continent has a large amount of land area, will favor the deposition in soil compartments, and as lead tends to deposit in this compartment, this will result in the higher value of FF in this region. But what is contributing, on a larger scale, to this result, is not the land area but the rain rate. Since this rate is higher in the Latin American region when compared to the African continent, this results in greater degradation and a lower persistence of lead in the soil. Also, the transport of lead by the action of rain to other compartments, where the persistence of this substance is lower, contributes to this result. Therefore, a lower FF value associated with the Latin American region is observed.

The iF values showed more significant differences since parameters such as the population determine, on a large scale, the exposure to the emission of a given substance. That is, the larger the population, the higher the exposure, resulting in a higher total iF. The production based-intake rates have also proved to be important for the calculation of this factor since they determine the exposure routes where the substance may be present. For example, considering again a lead emission, this time in natural soil: this substance presents the main intake route in almost all regions for the above-ground production exposure. However, in the Northern European and Oceania regions, the main route of lead intake is clearly through the consumption of fish. This is mainly due to differences in consumption patterns in each region and also the inherent characteristics of lead. Lead is a substance with a very large bioaccumulation factor in fish, indicating that the concentration in this organism is greater than of the medium from which this substance was released. Being Northern Europe and Oceania two regions with a much higher fish consumption than the rest, this will result in a high iF value for this intake route.

Due to these results, it was explored whether the model is, in fact, sensitive to site-specific parameters and it was concluded that the parameters related to human population and production-based intake rates had a greater influence on the calculation of XFs.

In conclusion, the influence of these parameters proved to be promising in the results presented, that is, site-specific parameters are necessary to take into account for the quality and accuracy of the LCIA results. The life-cycle toxicological impact assessment method USEtox revealed that it had the ability to be used to calculate the characterization factors of different substances and assess local toxicological impacts of substance emissions.

The LCA methodology, as mentioned before, usually neither addresses site-specific impacts nor impacts dynamic with time. This methodological limitation can be overcome with the inclusion of different scenarios dependent on time and location in order to create eco-regions that simulate the site-specific conditions of different training sites for several countries. The eco-regions are implemented in the USEtox model to predict the toxicological impacts for that specific characteristic. This information can help decision makers, with the inclusion of other complementary tools, to manage facilities like shooting ranges in a sustainable way.

5.2. Topics for future research

Since the main subject of this thesis, is the calculation and assessment of characterization factors for human toxicological and freshwater ecotoxicological impacts of chemical emissions, an interesting topic for future research could be the modelling of a shooting range using the USEtox model, and to study the behaviour of substances emitted in this space. Its modelling could be done using the site-specific environmental characteristics of a previously selected shooting range, varying only the relevant site-specific parameters for this space. The interest of this would be to understand whether it is possible to model a small space in the USEtox model, when compared to the continental or global scale. The subsequent analysis of the characterization factors of substances, allows to draw conclusions on this subject.

Another interesting topic to address in the future is the assessment of impacts resulting from chemical emissions, using the USEtox model. In this thesis, the analysis was made at the level of mid-points CFs. An emission compartment-specific toxicity impact score is calculated by multiplying the mass of a substance emitted in a given compartment with the corresponding toxicity midpoint or endpoint characterization factor. This impact becomes not only dependent on the chemical characteristics of the substance and the site-specific parameters, but also on the amount that is emitted, resulting in the contribution of this substance to the human toxicological and ecotoxicological impact categories.

To enhance the life-cycle studies about substances emission contamination, it is important to address in the future an important issue, related with the degradation of the substances when released in the environment that need to be accounted. These substances when reach the water or soil are not immutable and new substances arises from biotic or abiotic degradation, resulting in different organic or inorganic chemicals. These substances can have a different behaviour and, as a consequence, different potential toxicological impact from the originals emitted, so the assessment of the toxicological impact associated with the degradation of products is of great importance. The issue is to recognise which are the degradation products and the percentage rate of that degradation; nevertheless, some work has been evaluating these difficulties that can be used in the future to complete the life-cycle studies of substance emission contamination.

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ANNEX A: USETOX SITE-SPECIFIC PARAMETERS

Table A1. Described regions in USEtox model.

ID	Name
W1	Central Asia
W2	Indochina
W3	Northern Australia
W4	Southern Australia & New Zealand
W5	Southern Africa
W6	North, West, East & Central Africa
W7	Argentina+
W8	Brazil+
W9	Central America+ & Caribbean
W10	USA & Southern Canada
W12	Northern Europe & Northern Canada
W13	Europe
W14	East Indies & Pacific
IND	India+
CHI	Eastern China
JAP	Japan & Korean peninsula
North America	North America
Latin America	Latin America
Europe	Europe
Africa+Middle East	Africa & Middle East
Central Asia	Central Asia
Southeast Asia	Southeast Asia
Northern regions	Northern regions
Oceania	Oceania

Table A2. USEtox site-specific parameters and units for the continental scale.

Continental scale	**Area**	land	km^2
	Area	sea	km^2
	Areafrac	fresh water	[-]
	Areafrac	nat soil	[-]
	Areafrac	agr soil	[-]
	Areafrac	other soil	km
	Temp		ºC
	Surface wind speed		m.s^{-1}
	Wind speed over mixing height		m.s^{-1}
	Rain rate		mm.yr^{-1}
	Depth	fresh water	m
	Fraction fresh water discharge	cont-global	[-]
	Fraction run off		[-]
	Fraction infiltration		[-]
	Soil erosion		mm.yr^{-1}
	Irrigation		km^3

Table A3. USEtox site-specific parameters and units for the global scale.

Global scale	**Area**	land	km^2
	Area	sea	km^2
	Areafrac	fresh water	[-]
	Areafrac	nat soil	[-]
	Areafrac	agr soil	[-]
	Areafrac	other soil	km
	Temp		ºC
	Surface wind speed		m.s^{-1}
	Wind speed over mixing height		m.s^{-1}
	Rain rate		mm.yr^{-1}
	Depth	fresh water	m
	Fraction fresh water discharge	cont-global	[-]
	Fraction run off		[-]
	Fraction infiltration		[-]
	Soil erosion		mm.yr^{-1}
	Irrigation		km^3

Table A4. USEtox site-specific parameters and units for the urban scale.

Urban scale	**Area**	land	km^2
	Areafrac	Unpaved area	[-]
	Areafrac	Paved area	[-]

Table A5. USEtox site-specific parameters and units for human exposure.

Exposure	**Human breathing rate**	world + cont + urban	m^3/(person·day)
	Water ingestion	world + cont	l/(person·day)

Table A6. USEtox site-specific parameters and units for production-based intake rates.

ProductIon-based Intake rates	**Above-ground produce**	world	kg/(day·capita)
	Above-ground produce	continent	kg/(day·capita)
	Below-ground produce	world	kg/(day·capita)
	Below-ground produce	continent	kg/(day·capita)
	Meat	world	kg/(day·capita)
	Meat	continent	kg/(day·capita)
	Dairy products	world	kg/(day·capita)
	Dairy products	continent	kg/(day·capita)
	Fish freshwater	world	kg/(day·capita)
	Fish freshwater	continent	kg/(day·capita)
	Fish coastal marine water	world	kg/(day·capita)
	Fish coastal marine water	continent	kg/(day·capita)

Table A7. USEtox compartments.

ABBREVIATION	COMPARTMENT
home.airI	Household indoor air
occ.airI	Occupational indoor air
airU	Urban air
airC	Continental rural air
fr.waterC	Continental freshwater
sea.waterC	Continental sea water
nat.soilC	Continental natural soil
agr.soilC	Continental agricultural soil
airG	Global air
fr.waterG	Global freshwater
oceanG	Global ocean
nat.soilG	Global natural soil
agr.soilG	Global agricultural soil

ANNEX B: USETOX SUBSTANCE PARAMETERS

Table B1. Chemical parameters values and units used in USEtox for the calculation of the toxicological characterization factors of the selected substances.

	Substance					
Parameter	**Formaldehyde**	**Allyl alcohol**	**Octane**	**Lead**	**Dioctyl terephthalate**	**Unit**
PesticideTargetClass	Fungicide					-
PesticideChemClass	Other class					-
MW	3.00E+01	5.81E+01	1.14E+02	2.07E+02	3.90E+02	$g.mol^{-1}$
pKaChemClass	neutral	neutral	neutral			-
pKa.gain						-
pKa.loss						-
K_{OW}	2.24E+00	1.48E+00	1.51E+05		6.46E+07	$L.L^{-1}$
Koc					3.97E+05	$L.kg^{-1}$
K_{H25C}	3.40E-02	5.04E-01	3.24E+05	1.00E-20	9.75E+02	$Pa.m^{3}.mol^{-1}$
Pvap25	5.19E+05	3.48E+03	1.88E+03	2.40E-23	1.00E-03	Pa
Sol25	4.00E+05	1.00E+06	6.60E-01		4.00E-04	$mg.L^{-1}$
K_{DOC}				4.79E+06	5.17E+06	$L.kg^{-1}$
Kp_{SS}				7.48E+06		$L.kg^{-1}$
Kp_{Sd}				3.98E+04		$L.kg^{-1}$
Kp_{Sl}				2.00E+03		$L.kg^{-1}$
$kdeg_{A}$	7.03E-06	1.94E-05	6.51E-06	1.00E-20	2.41E-05	s^{-1}
$kdeg_{W}$	5.35E-07	5.35E-07	9.25E-07	1.00E-20	7.72E-07	s^{-1}
$kdeg_{Sd}$	5.94E-08	5.94E-08	1.03E-07	1.00E-20	9.53E-09	s^{-1}
$kdeg_{Sl}$	1.34E-06	2.67E-07	4.63E-07	1.00E-20	1.93E-07	s^{-1}
$kdiss_{P}$	6.15E-06	6.36E-06	5.31E-06			s^{-1}
$kdiss_{wheat}$	9.30E-06					s^{-1}
$kdiss_{rice}$	4.66E-06					s^{-1}
$kdiss_{tomato}$	6.59E-06					s^{-1}
$kdiss_{apple}$	5.23E-06					s^{-1}
$kdiss_{lettuce}$	1.31E-05					s^{-1}
$kdiss_{potato}$	1.04E-05					s^{-1}
$av_{logEC50}$	1.49E+00	-6.20E-03	-2.26E+00	-2.14E+00	6.56E-02	$log(mg.L^{-1})$
$ED50_{inh,noncanc}$	5.90E+01	9.44E+00		5.79E-02	5.00E+03	$kg.lifetime^{-1}$
$ED50_{ing,noncanc}$	5.90E+01	9.44E+00		5.79E-02	5.00E+03	$kg.lifetime^{-1}$
$ED50_{inh,canc}$	4.71E-01			2.03E+01		$kg.lifetime^{-1}$
$ED50_{ing,canc}$	2.43E+02	NEG		2.03E+01		$kg.lifetime^{-1}$
BAF_{root}				3.00E-03		$kg_{veg}.kg_{soil}^{-1}$
BAF_{leaf}				1.10E-02		$kg_{veg}.kg_{soil}^{-1}$
BTF_{meat}				7.00E-04		$d.kg_{meat}^{-1}$
BTF_{milk}				1.90E-04		$d.kg_{milk}^{-1}$
BAF_{fish}	1.06E+00	9.92E-01	1.16E+03	3.70E+02	3.23E+06	$L.kg_{fish}^{-1}$