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OMNIITOX Base Model Sensitivity Analysis Toward Nature Framework Properties

Master's Thesis

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CHALMERS UNIVERSITY OF TECHNOLOGY
Environmental Systems Analysis
Göteborg, Sweden, 2005
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Abstract

This thesis attempts to analyse the sensitivity of the OMNIITOX base model by identifying the influence of nature framework properties on characterisation factors. The base model calculates characterisation factors representing toxic impacts on human health and ecosystem. To calculate the characterisation factors this model is using substance property values and nature property values as input values. The model to calculate the characterisation factors uses a dynamic calculation matrix, which is influenced by those input values significantly. The motivation of this work was to observe the influenced of nature property values on base model. To do so several task have been done. In OMNIITOX base model the Globe is divided into Europe and World (rest of Europe). In this work a new system boundary was specified among the European countries. Europe was defined as EU-25 countries, Norway, Switzerland, Iceland plus two EU candidate countries Bulgaria and Romania. In addition nature framework properties are not well defined in OMNIITOX documentation. So we tried to define the nature framework properties and data were gathered for the prioritised properties. Finally, characterisation factors were calculated by giving input the new and old data sets into the OMNIITOX IS and then the results were compared in plots.

This work shows that impacts on human health and ecosystem are influenced by nature property values in case of Europe as the data were gathered for Europe. Some irregular characterisation factors; for substance CAS number 309-00-2, 87-68-3; and unexpected negative characterisation factors; for substance CAS number 7440-43-9; were observed during the calculation for new data set. Quantitatively most of the new data are larger than the old ones and from the regression lines we observe that the influence of new nature property values is dominating over old nature property values for both ecotoxicity impact factor and human damage factor. The only exception is for human damage factor agricultural soil emission Europe. Because of complex calculation matrix we could not find out the reason for such unusual behaviour of characterisation factors. Reliability and acceptance of results for such a multimedia model is a crucial issue. In addition the output of an operational model like OMNIITOX base model should be acceptable and clearly understandable to its users. Limitations of this analysis can be considered for further sensitivity analysis of this model taking into consideration more nature property data and more substances.

Key words: Sensitivity, Nature framework property, Characterisation factor, System boundary, CAS number.

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1. Introduction

The OMNIITOX (Operational models and information tools for industrial applications of eco/toxicological impact assessments) base model is a comprehensive and relatively complex environmental fate and exposure multi-media model. It was developed in OMNIITOX-project to calculate the characterisation factors for the most commonly used chemicals. The model core calculates the characterisation factor for human toxic effects and the characterisation factor for ecotoxicological effects. The base model constitutes several modules containing specific models for chemical fate, human exposure and human health/ecosystem effects, linked via a model core. The modules comprise the fate compartments: air, fresh water + sediment, marine water + sediment, soil, vegetation as well as modules for human exposure, human health effects and ecotoxicological effects. This model has applied a specific geographical system boundary representing various nature framework data. In OMNIITOX nature framework concept refers to system frame models of the environment. Nature frameworks have system boundaries and nature properties such as geographical, hydrological, biophysical, meteorological etc.

The aim of this thesis work is to analyse the sensitivity of the base model for various choices of system boundaries of the fate and exposure parts. This is a preliminary attempt to investigate the influence of nature framework properties on base model sensitivity. How much the characterisaiton factors are changed that is the interest of this analysis. To perform the analysis specification of new system boundary and data gathering for the prioritised nature framework properties have been done. Political boundaries were chosen to specify the new system boundary due to data availability. In addition prioritised nature properties were defined to gather reliable data. The calculations have been carried out in OMNIITOX information system and the results were compared.

The rest of the report presents OMNIITOX concept model, OMNIITOX information system, methodology in details, discussion of results and finally concluding remarks.

2. OMNIITOX concept model

The concepts load, indicator, mechanism, nature framework, and substance are the cornerstones in the OMNIITOX concept model, figure 2.1 (Tivander et al., 2004, p-10). In addition to the core concepts a number of concepts have been defined to support the core. This includes in particular the structuring of substance property data, a flexible structure to handle quantitative data and quality meta data, a knowledge base for reference documentation, etc. (Tivander et al., 2004)

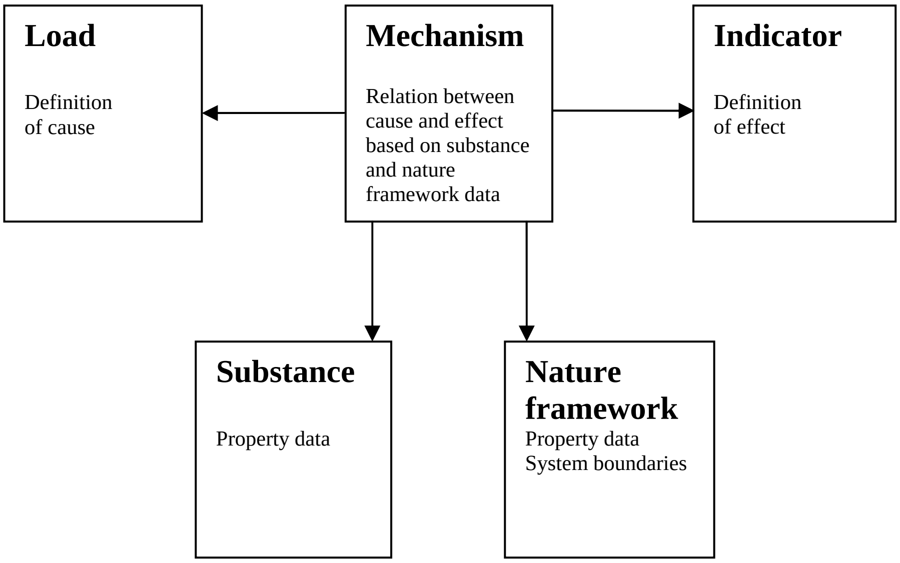

Figure 2.1: The core of the OMNIITOX concept model.

2.1 Substance and Nature framework

The substance property specification concept is equivalent to substance property type in the OMNIITOX data format. A substance property type is not inherently connected to any specific substance, but it describes the aspects of the property that is common to all applicable substances, i.e. the description of its physical representation, the acceptable acquisition method(s) to obtain substance properties, etc.

The nature framework is in general a specification of chosen system boundaries and system conditions for a model of the nature system. Nature frameworks have system boundaries and nature properties that are independent of substances. System boundaries and internal distribution of compartment media, geography, time frame, etc. can be specified. It is possible to specify borders between nature frameworks on any given dimension. Nature Framework Property Type is used to define properties in the nature system. In OMNIITOX this is called Nature Framework Property Specification.

2.2 OMNIITOX Information System

OMNIITOX information system is a platform for calculation of characterisation factors to be used in an LCA context. It has been developed primarily to facilitate characterisation modelling and calculation of characterisation factors representing toxic impact. For model transparency and consistency OMNIITOX IS requires the documentation of the model data that should contain mathematical representation as well as a qualitative description of characterisation models to calculate the characterisation factors.

OMNIITOX information system contains substance data (includes substance names and substance property specifications), nature data (includes nature frameworks and nature property specifications) and characterisation models (calculate characterisaiton factors). In addition the information system contains nomenclature and a knowledge base containing manuals for user and interpretation support, a list of related data sources and related reports etc.

Nature property values have been inserted into the database for the nature framework “Global” consisting of “Europe” and “World (rest of Europe)”. For nature properties there are seven different categories: Biophysical, Geographical, Constant, Geological, Hydrological, Meteorological, and Production. On the other hand, for substance properties there are five different categories: Chemical-physical; Fate, transport and transformation; Human toxicological; Ecotoxicological; and Model control.

Substances may have many synonymous names and many various properties. Every substance property is derived by a specific model that involves aggregation of data. The value may be relative or absolute, be quantitative or qualitative, and based on calculations and/or value choices. Some substance property values are dependent on ambient conditions at the measurement. It may hence be necessary to specify more than one substance property parameter to sufficiently document the substance property. The substance property concept encompasses not only the value of the property but also a description of the actual acquisition method applied to obtain the value. A specific substance property may have more than one value from different data sources. Substance property specification describes all these information. Nature properties are defined similarly as in the substance concept.

OMNIITOX IS has described the same data documentation format for all substance and nature properties. This property specification documentation format is presented in the following table 2.1. (OMNIITOX 2003)

Table 2.1: Data documentation format for substance and nature property specifications.

Default name	The descriptive name of the property.
Alternate name	Other (common) names used for the same property.
Category	Select the category of the substance property from the nomenclature, e.g. “Chemical/Physical” or “Toxicological”.
Physical representation	An explanation of what the property represents.
Condition	The condition specifies the explicit dependency of the property, e.g. type of soil, temperature, compartment etc. A condition value can be of three types: quantitative, classifying, or qualitative. Each classifying condition, e.g. Type of soil, Test species, Zones etc. has to be specified with a nomenclature, e.g. [Clay; Clay loam; Silt loam;…]. The condition/conditions, unit/units and value type/value types are stated here, separated with semicolon if several, e.g. Type of soil [N/A; classifying]; Temperature [°C; qualitative]; …
Standardized method for property specification	If the property value have to be acquired with a standardized method, please select the method from an OMNIITOX nomenclature with standardized methods, e.g. - Testing Methods of Annex V to Directive 67/548/EEC at the European Commission (http://www.europa.eu.int or http://ecb.jrs.it) or - OECD Guidelines for the testing of chemicals at OECD (www.oecd.org) - … - Other If other methods are accepted, you should select “Other” in the nomenclature. Other methods may be further described in “Method description…” below, but it will not imply any real requirements for the property values.
Method description for property specification	If there are other methods accepted, than the ones standardized according to OMNIITOX nomenclature, they may be described in this field. Please note that if the information in this field is contradictory to the selected standardized method in the property specification, the standardized method will be valid for the property in the information system.
Date for property specification	In this field the relevant date or dates for the data acquisition, documentation etc. should be entered. All dates should be specified with a comment on in what way the information was treated (acquired, up-dated, documented in OMNIITOX IS etc) at this time.

Value type	The value type for the property can be quantitative, classifying, or qualitative. Each classifying property value, e.g. “Mutagenicity based on salmonella or E.Coli bacteria” has to be specified with a nomenclature, e.g. [Mutagenic; Non-mutagenic; Ambiguous].
Unit	The unit of the property that is valid in OMNIITOX IS is stated in this field. Only one unit can be stated here. If other units are applicable they can be stated in the Unit specification field and any guidelines for re-calculation can also be described in that field.
Unit specification	An explanation of the unit can be given here, or instructions for how to recalculate the unit into other units manually.
Reference for property specification	The reference or references to the sources of information used to describe the property specification are stated in this field. The reference field should contain a numbered reference list with complete references. The numbers should be stated in square brackets, starting with the reference appearing firstly in the data documentation format, and the rest in consecutive order. A complete reference should be made so that the data source can be found without contacting the author of the substance property, i.e. involving title of report/ book/database etc, number/version, name of responsible company/author, address/city/country/web address, year etc.
Modeller	The person or persons that have modelled and documented the property should state their name and address in this field. If there are several persons involved in the modelling and documentation, it may also be specified who has done what.
Applicability	Information about how this property is or can be applied is stated in this field.

3. Methodology

The OMNIITOX base model provides characterization factors for a limited number of well investigated substances. Because the substance properties required for the base model is 47, i.e. about 47 data sets have to be acquired for each substance to get characterization factor(s). To investigate the influence of nature framework properties on characterisation factors a new system boundary was specified depending on political boundary among the European countries. Country level data availability is one of the reasons for choosing political boundary. Europe has been defined as EU-25 countries, Norway, Switzerland, Iceland plus two EU candidate countries Bulgaria and Romania. Greenland is excluded from the area of Denmark.

As this work will compare the results between two system boundaries so area dependency was given high priority during prioritisaiton of nature framework properties. In addition data availability and environmental impacts were also considered. Nature framework properties (NFP) are not well defined in OMNIITOX documentation as well as in OMNIITOX information system. Prioritised NFP were defined so that the users can understand what is meant by the property exactly.

In the nature property data template 141 values were given. Among them 34 nature properties, see in appendix, were primarily chosen for data gathering. Data have been gathered for these prioritised nature properties within the newly specified geographical system boundary keeping all other values constant. Finally values for 19 nature framework properties were obtained from various sources and implemented in the OMNIITOX IS. Characterisation factors (CF) of new data set and old data set were calculated for 19 substances (see appendix) and CFs have been compared.

3.1 Fate compartments

Different chemicals have different fates in the environment. Some may accumulate in the compartment into which they are released; e.g., heavy metals released into surface water tend to accumulate in the sediments. Other chemicals may physically, chemically, or biologically be transformed through processes such as hydrolysis, oxidation, or biodegradation. Certain contaminants may move into another compartment through processes including advection, volatilization, and precipitation. Therefore, human exposure and human health/ecosystem effects are depending on the characteristics of fate compartments. The OMNIITOX base model core constitutes models for chemical fate in different compartments. So primarily it has been tried to distinguish the environmental media of the new geographical system boundary by collecting country level data from national statistical databases. But unavailability of data has become a problem. Data reliability is another concern for country level data as the parameters are not well defined and also data acquisition methods are not documented in most cases. To solve this problem several reliable data sources have been chosen like CIA factbook, Eurostat, European Environment Agency (EEA), United Nations Environment Programme (UNEP), World Resources Institute (WRI), Food and Agriculture Organizaiton (FAO) etc.

In this thesis work area total is defined as the sum of area of soil compartment, area of fresh water compartment and area of sea water compartment i.e., continental shelf area whereas in OMNIITOX it is according to the fraction of the ocean area. During this analysis area of ocean compartment is excluded from the area total of Europe due to several reasons, which is discussed in the sea compartment.

3.1.1 Soil compartment

Soil is the most heterogeneous medium among all the media considered in a multi-media model. In this thesis work soil area is defined as the area of soil compartment. According to CIA factbook soil area aggregates all surfaces delimited by international boundaries and/or coastlines, excluding inland water bodies; lakes, reservoirs and rivers. The area of soil compartment Europe was calculated by aggregating the country level data taken from the CIA factbook 2004 for all the countries considered under new system boundary. The value obtained from the calculation is 4.639E+12 m2, which is 1.5 times greater than the old value.

Area of soil compartment includes the natural soil compartment and agricultural soil area. The distinction of agricultural soil is necessary for the sake of exposure assessment. Agricultural area is the sum of area under arable land, permanent crops and permanent pastures (FAO 2001). Arable land is the land under temporary crops; double-cropped areas are counted only once; temporary meadows for mowing or pasture, land under market and kitchen gardens and land temporarily fallow; less than five years. The abandoned land resulting from shifting cultivation is not included in this category. Permanent crops land cultivated with crops that occupy the land for long periods and need not be replanted after each harvest, such as cocoa, coffee and rubber; this category includes land under flowering shrubs, fruit trees, nut trees and vines, but excludes land under trees grown for wood or timber. Permanent pasture land used permanently; five years or more; for herbaceous forage crops, either cultivated or growing wild; wild prairie or grazing land. The dividing line between this category and the category "Forests and woodland"; is rather indefinite, especially in the case of shrubs, savannah, etc., which may have been reported under either of these two categories.

In this model agricultural soil area is defined as the area of agricultural soil compartment. Country level data have been adapted from the FAOSTAT and then aggregated. Surface area of natural soil compartment was calculated by using the following formula, which is adapted from the OMNIITOX documentation. Area of natural soil compartment = Area total – Area of ocean compartment – Area of seawater compartment – Area of fresh water compartment – Area of soil compartment. The calculated new values are significantly bigger compared to the old values and this is clearly because of the addition of several new countries in the new system boundary. Table 3.1 shows the comparative values of area of soil compartment, area of agricultural soil compartment and area of natural soil compartment for both the system boundaries.

Table 3.1: Area of soil compartments under old and new system boundaries.

Nature property parameter	**Unit**	**Old value**	**New value**
Area of soil compartment	m2	3.08E+12	4.639E+12
Surface area of agricultural soil compartment	m2	1.5E+12	2.045E+12
Surface area of natural soil compartment	m2	1.58E+12	2.59E+12

3.1.2 Fresh water compartment

Inland water bodies play an important role in the transportation of toxic chemicals. A chemical in water distributes between particulate matter, colloidal organic matter and dissolved phases. The distribution over these phases determines their availability for different processes leading to degradation and to transfer processes to other compartments, like volatilisation to air, deposition to sediment or advection to the ocean. In addition, chemicals dissolved in water can also be transferred to sediment via diffusion processes. So it is very important to define the area of fresh water compartment. In CIA factbook water area is defined as the sum of all non-salt water surfaces delimited by international boundaries and/or coastlines, including inland water bodies; lakes, reservoirs, and rivers. Country level values of water area, which is considered as area of fresh water, were taken from the CIA factbook 2004 and the values were aggregated to obtain the area of fresh water Europe.

Abstracted freshwater in Europe is used for urban use (14%), agriculture (30%), and industry (10%, cooling water excluded), and for cooling water for power generation and hydropower (32%), and other or undefined uses (14%).

Agricultural water use and water use productivity is not always available at country level. If such data exist, they are in most cases not very reliable. This is mainly due to the complexity of the assessment methods and to the absence of direct measurement of water withdrawal for agriculture. As they are among the most crucial indicators in assessing progress in agricultural water use, a review of countries' agricultural water use is necessary to improve the overall quality of global water resources monitoring (FAO 2005). Renewable water resources available to irrigation and other uses are commonly defined as the part of precipitation which is not evaporated or transpired by plants, including grass and trees, which flows into rivers and lakes or infiltrates into aquifers. The annual water balance for a given area in natural conditions, i.e. without irrigation, can be defined as the sum of the annual precipitation and incoming flows; transfers through rivers from one area to another; minus evapotranspiration.

One of the biggest driving forces and pressures on water resources is agriculture and the changes in its practices. Production rate of irrigation water is calculated from the amount of water used in the agricultural sector per square kilometer of arable and permanent cropland in the year specified. Irrigation is the primary use of water in the agricultural sector. To estimate the pressure of irrigation on the available water resources, an assessment has to be made both of irrigation water requirements and of water withdrawal for agriculture. Data on country level water withdrawal for agriculture have been collected through AQUASTAT 2001 country surveys. Data on water requirement ratios are generally not easily available at field, irrigation scheme or river basin levels. At country level, only very scattered and unreliable information is available. For this reason, it is better to use a regional rather than national approach to assess water requirement ratios. (FAO 2005)

Mean air temperature plays an important role in direct and indirect human exposure to toxic chemicals. Increase in temperature may increase the volatilisaiton of semi-volatile compounds. Estimations of climate change indicate a temperature increase of 1º C to 3.5º C by 2100, which together with an increase in precipitation in Northern Europe and a decrease in Southern Europe, could lead to a reduction in renewable water resources in Southern Europe. Furthermore, a temperature increase could cause snow to melt earlier, increasing winter run-off and reducing the thawing processes in spring and summer. Even in areas where precipitation increases, greater evaporation could lead to lower run-off. Climate change may have considerable repercussions on the flood regime (Krinner et al., 1999). Mean air temperature is the double average over space and time. Country level 'mean air temperature' is not available for all the countries within the new system boundary. In those cases it was calculated from the average temperature of different measuring stations of a country.

Precipitation rate is calculated from average precipitation which is the double average over space and time of water falling on the country in a year, referring to a given reference period. Country level yearly average precipitation for the period 1961 – 1990 is given in AQUASTAT. The calculated precipitation rate of new system boundary is 0.002318 m/day.

Groundwater provides 70% of Europe's drinking water, supplying around 300 million people. Groundwater Recharge is defined as the total volume of water entering aquifers within a country's borders from endogenous precipitation and surface water flow. Natural incoming flows originating from outside a country's borders are not included in the total. Throughout the world, regions that have sustainable groundwater balance are shrinking day by day. Three problems dominate groundwater use: depletion due to overdraft; water logging and salinisation due to inadequate drainage and insufficient conjunctive use; and pollution due to agricultural, industrial and other human activities. In many regions of the world, especially with high population density, dynamic tube-well-irrigated agriculture and insufficient surface water, many consequences of groundwater over development are becoming increasingly evident. The most common symptom is secular decline in water tables. In many areas artificial recharge of ground water have been done to reduce the adverse effect on ecosystem and human health.

Table 3.2 shows the values of nature property parameters that are affecting the fresh water management system and/or dependent on the fresh water compartment and also shows a comparison between old and new values.

Table 3.2: Comparative nature framework property values.

Nature property parameter	**Unit**	**Old NFP value**	**New NFP value**
Surface area of fresh water compartment	m2	1.08E+11	1.55E+11
Precipitation rate	m/day	0.00136	0.002318
Production rate of irrigation water	m3/day	249000000	292616164
Rate of ground water recharge	m/day	0.0000114	0.00026955
Mean air temperature	K	281	282.4

3.1.3 Sea water compartment

In OMNIITOX base model the marine ecosystem, which is the single largest ecosystem of the world, is subdivided into two compartments, sea and ocean compartment. Continental shelf area is considered as surface area of sea water compartment in this thesis work. According to the United Nations Convention on the Law of the Sea (UNCLOS), the continental shelf area is defined as the area of the sea bed and subsoil which extends beyond the territorial sea to a distance of 200 nautical miles from the territorial sea baseline and beyond that distance to the outer edge of the continental margin. Areas of continental shelf that are disputed by overlapping claims by one or more nations have been excluded from this table. Areas that are of cooperative joint development between two or more nations have also been excluded. Coastal states have sovereign rights over the continental shelf; the national area of the seabed; for exploring and exploiting it. The shelf can extend at least 200 nautical miles from the shore, and more under specified circumstances. The UNCLOS is an international agreement that sets conditions and limits on the use and exploitation of the oceans. This Convention also sets the rules on how the maritime jurisdictional boundaries of the different member states are set.

Biogeochemical processes principally occur in the upper 200 metres of the sea and are often associated with continental margins, with water shallower than 200 m, occupy a mere 7% of the ocean surface and even less than 0.5% of the ocean volume, they still play a major role in oceanic biogeochemical cycling. Significantly higher rates of organic productivity occur in the costal oceans than in the open oceans because of rapid turnover and the higher supply of nutrients from upwelling and riverine inputs (Chen, 2003).

According to marine geochemists environmental processes affecting organic and inorganic substances are most intensive in the shallow continental sea. In the continental seas most of the substances that have entered the sea by river transport are removed from the water column. Only a fraction of the substances that entered the sea through river transport will finally end-up in the oceans (Chester, 1990).

Subdivision of marine ecosystem is necessary for the above reasons. Ocean is considered as a sink of toxic substances because of much more longer residence time than costal seas. Ocean compartment is excluded from this work because of unavailability of country level data and lack of geochemical information.

Most of the coastal seas in this world are not connected to the European coastal waters (i.e. all the coastal waters alongside the North & South America, Asia, Oceania, Antartica). Therefore, we may assume that the exchange between European coastal waters and World average coastal waters is negligible and may be set to zero. The only way in which contaminants may enter the world average coastal waters from the European continent is by way of air. (Bachmann, 2004)

Values of different compartments in nature system under existing system boundary and newly specified system boundary are presented in the figure 3.1.

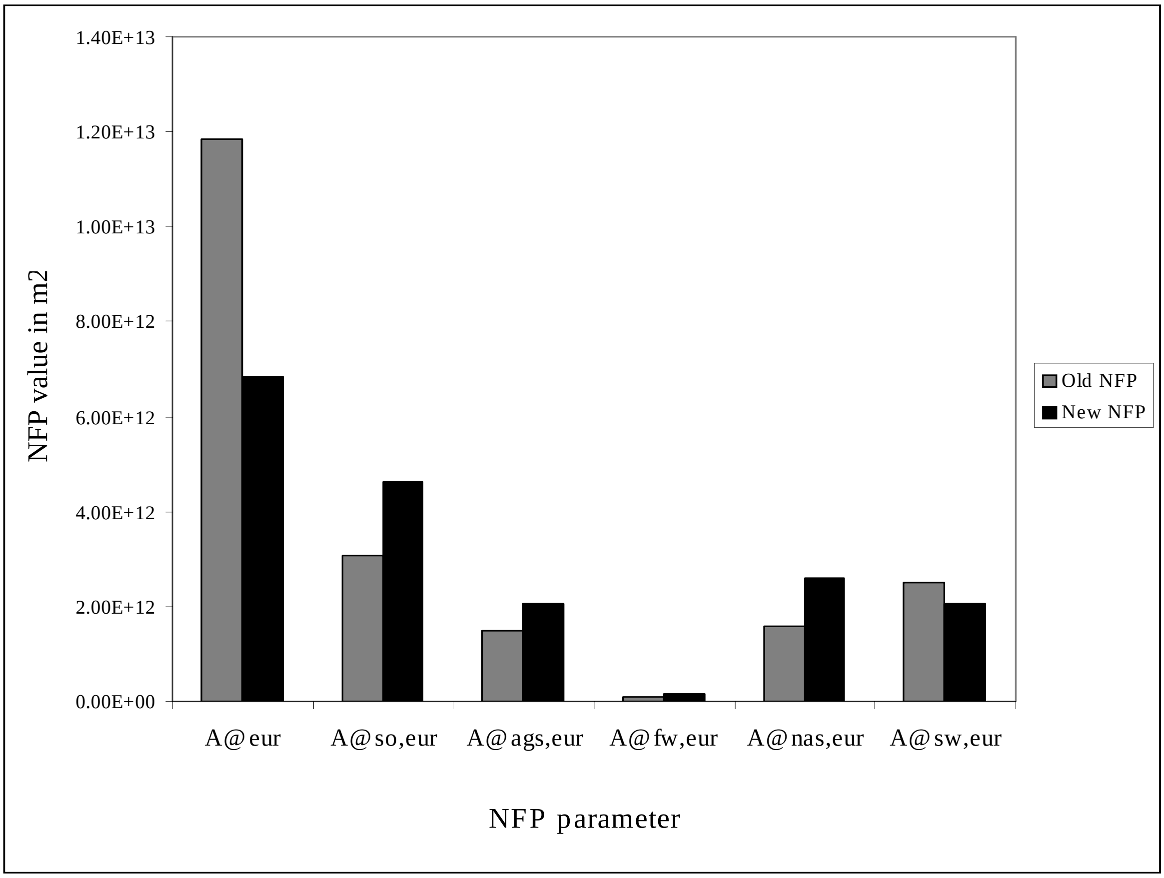

Figure 3.1: Area of different compartments in old and new system boundary. Here A@eur = area total Europe; A@so,eur = area of soil compartment Europe; A@ags,eur = area of agricultural soil compartment Europe; A@fw,eur = area of fresh water compartment Europe; A@nas,eur = area of natural soil compartment Europe and A@sw,eur = area of sea water compartment Europe.

The big difference in area total Europe is because of the exclusion of ocean compartment.

3.2 Production data

Human exposure to toxic chemicals can occur by direct and indirect pollutant intake from environmental media and via the consumption of intermediate exposure substrates; e.g., meat, milk, eggs, fish etc. Production data on animal; such as beef, pig, poultry, sheep; fisheries, egg, milk are taken from the Food and Agriculture Organisation statistical database for the year 2001. Country level ‘primary production data’ are given in FAO statistical database. Data on meat production are usually reported according to one or more of the following concepts: 1. Live weight of animals intended for slaughter is the weight taken immediately before slaughter. It is assumed that animals intended for slaughter are kept in the slaughterhouse premises for 12 hours and are not fed or watered during this time. 2. Killed weight is the gross weight of the carcass including the hide or skin, head, feet and internal organs, but excluding the part of the blood which is not collected in the course of slaughter. Production data for milk refer to raw milk containing all its constituents. Trade data normally cover milk from any animal, and refer to milk that is not concentrated, pasteurized, sterilized or other-wise preserved, homogenized or peptonized. (FAO 2001)

For production data, one would expect that the supply is usually larger than the consumption. This can be explained by the fact that not all food that is assessed to be available for consumption is finally eaten e.g., due to loss, plate-waste. Additionally, there are many gaps in deriving the food balance sheets (FBSs) particularly in the statistics of utilization for non-food purposes, which might lead to a reduction of the estimated per capita food supply. Within the assessment, it is assumed that 5 % of the food supply is lost in order not to overestimate the exposure. (Bachmann 2005)

In the base model the production data refer to the production of food per year in kg that is ready to be consumed by the total population. During calculation of production data an average 5% food loss value is subtracted from the total value though for all substrate the loss is not the same. Export-import data are excluded from production data due to unavailability of data though it plays an important role in human food consumption and exposure to the substances.

Changes in population, population distribution and density are key factors influencing the exposure of toxic substances which affecting the human health and ecosystem. Total population refers to the present-in-area population, which includes all persons physically present within the present geographical boundaries of countries at the mid-point of the reference period. The total population of Europe in the year 2001 is 4.94E+08. (FAOSTAT 2001)

Table 3.3 lists comparative production data for old and new system boundaries, which is shown in the figure 3.2.

Table 3.3: Production data for old and new system boundaries.

Nature property parameter	**Unit**	**Old value**	**New value**
Production rate beef	kg/yr	8.58E+09	8.03E+09
Production rate egg	kg/yr	6.34E+09	6.6E+09
Production rate fresh water fish	kg/yr	1.13E+08	2.73E+09
Production rate sea water fish	kg/yr	1.67E+09	8.48E+09
Production rate milk	kg/yr	1.46E+11	1.52E+11
Production rate pig	kg/yr	2.21E+10	2.08E+10
Production rate poultry	kg/yr	8.69E+09	1.06E+10
Production rate sheep	kg/yr	1.06E+09	1.05E+09

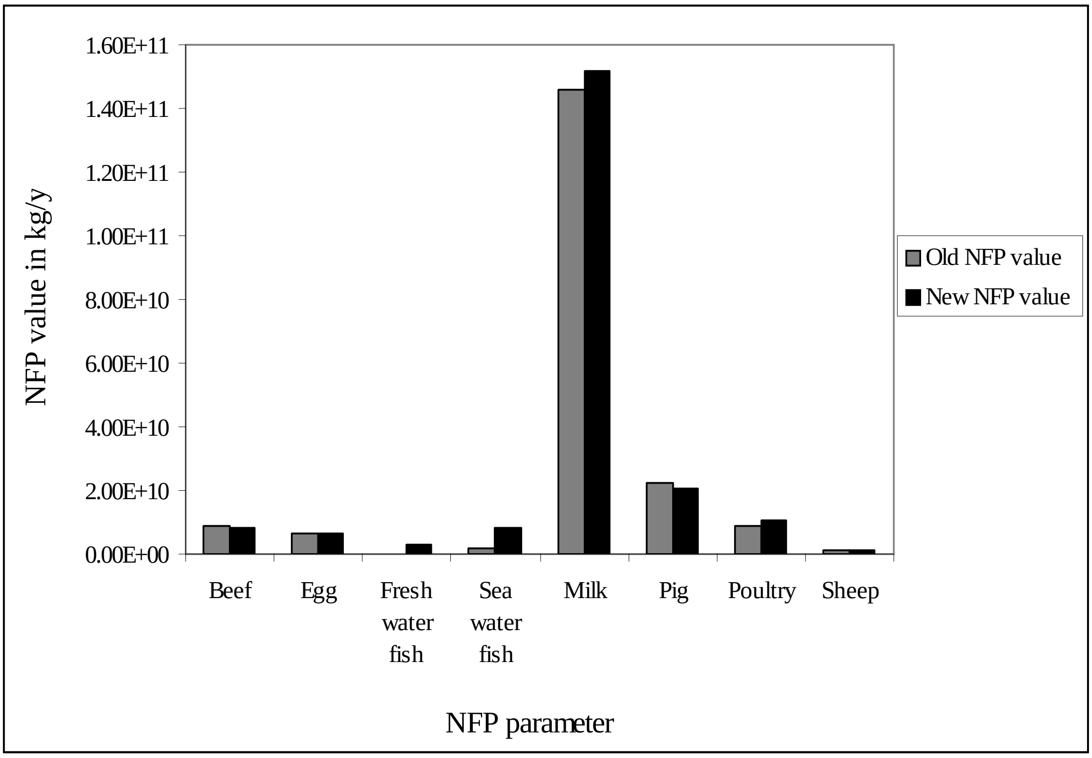

Figure 3.2: Production data for old and new system boundary.

From the above figure we can see that the difference in production data is not significant though the area of soil compartment, area of agricultural soil compartment and area of freshwater compartment of new system boundary are significantly bigger than those of old system boundary. This is probably due to the data acquisition methods and year of data acquisition used in the both systems.

3.3 Constant nature property parameters

In OMNIITOX model some constant parameters are used in constant category. The values are summarised in the table 3.4.

Table 3.4: Constant nature property parameters

Mechanism parameter	**Unit**	**Value**	**Description**
Junge equation constant	Pascal meter (Pa*m)	0.17	Pressure length
Mol weight water	gram per mole (g/mol)	18	Mass
Time dilution constant	Day	1	A transformation constant representing over how long time a time-concentration or time mass exists
Universal gas constant	pascal cubic meter per Kelvin mole (Pa*m3/K*mol)	8.31451	Universal gas constant

4. Result and discussion

OMNITOX base model calculates characterisation factors for toxic chemicals representing “Ecotoxicity impact factor” and “Human damage factor”. From the calculated characterisation factors we observe that the influence is minor in case of world whereas quite big for Europe with the change in nature framework property values. We predicted that the change in characterisation factors for World would be negligible as we kept the World data unchanged. For few substances new CFs are showing big difference compared to the old CFs in case of Human Damage Factor Europe. Some unexpected negative CFs are also observed for one substance; CAS number 7440-43-9. The calculated characterisation factors are compared in the following graphs both for ecotoxicity impact factor and human damage factor. The graphs show the CFs for old data set on the X-axis and for new data set on the Y-axis.

4.1 Ecotoxicity impact factor

The ecotoxicity impact factor describes the potentially affected fraction (PAF) for a species per kg emission (PAF*m3*year/kg). In the interpretation of the CFs of the OMNIITOX BM distinguishes three different pathways: air, fresh water and agricultural soil emission both for Europe and World. Figure 4.1, 4.2 and 4.3 represents the ecotoxicity impact factor air, freshwater and agricultural soil emission respectively for both Europe and World.

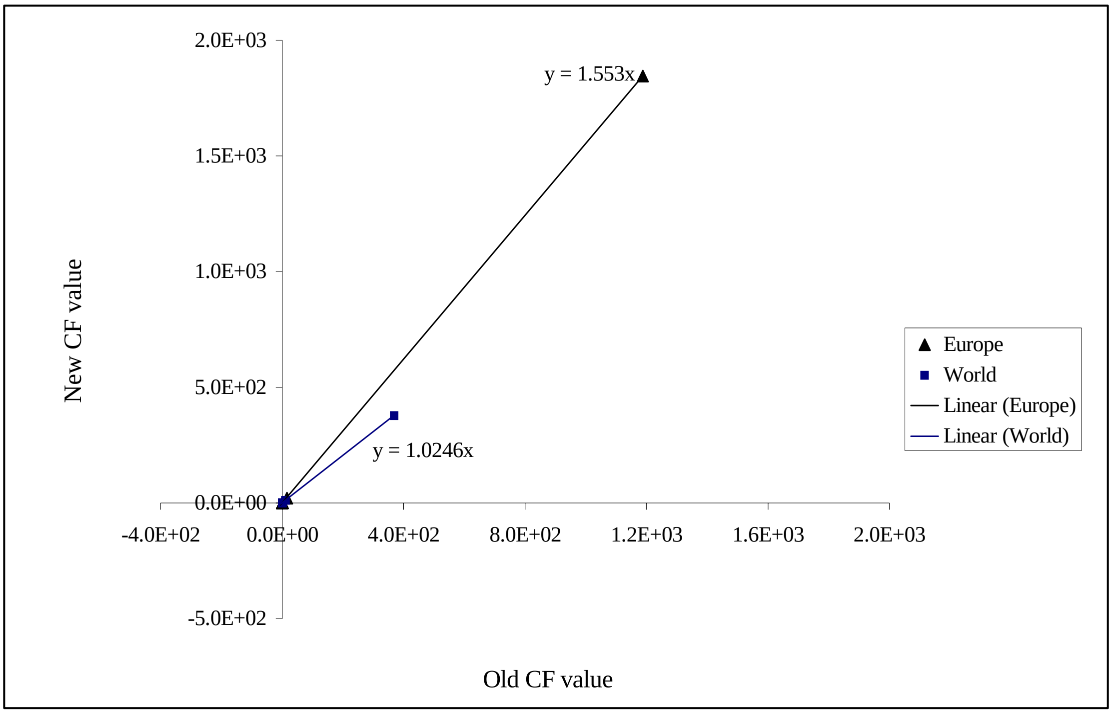

Figure 4.1: Fresh water ecotoxicity impact factor air emission Europe and World

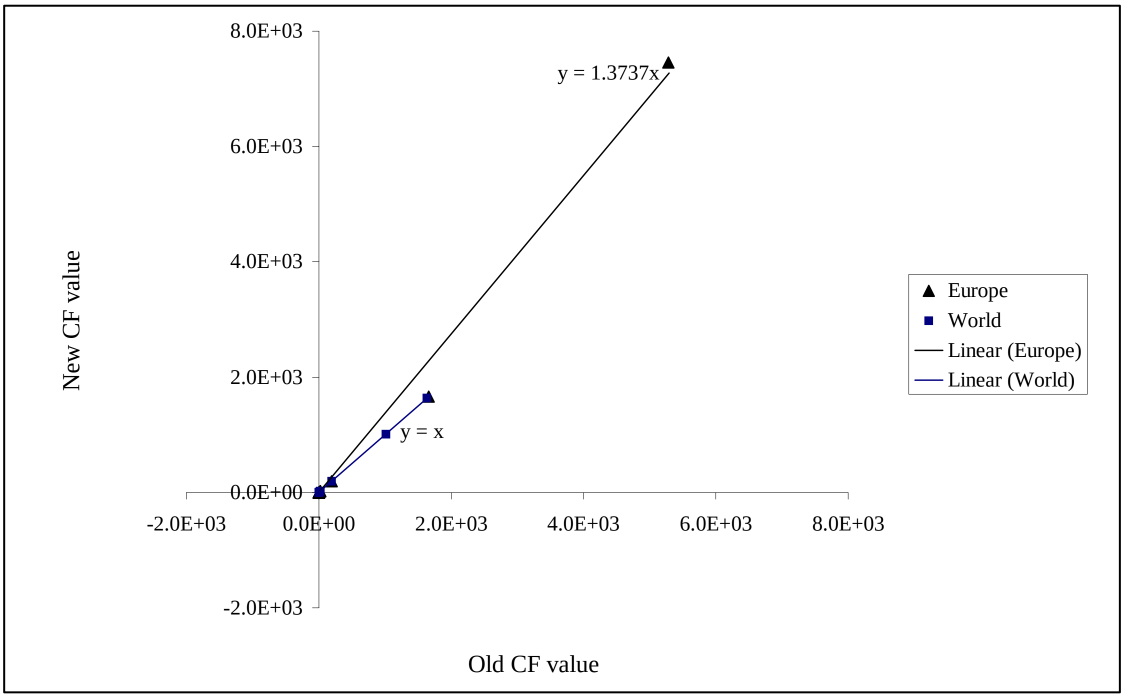

Figure 4.2: Fresh water ecotoxicity impact factor fresh water emission Europe and World

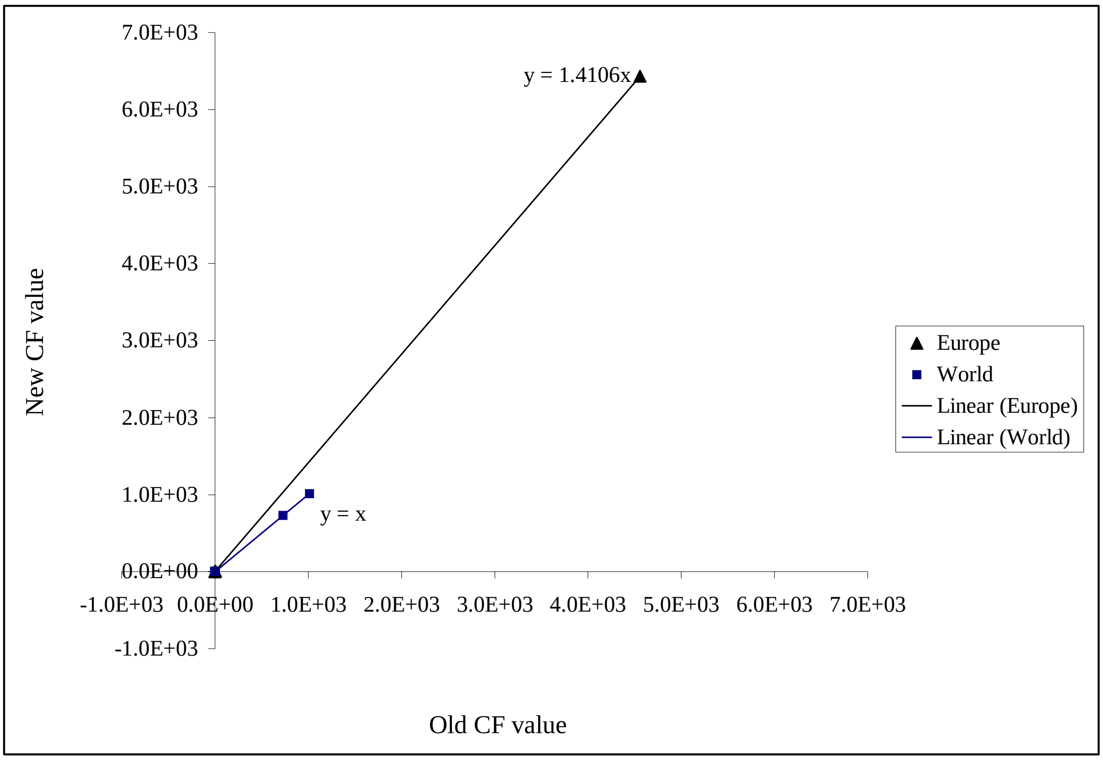

Figure 4.3: Fresh water ecotoxicity impact factor agricultural soil emission Europe and World.

Comparing the slope and square of correlation coefficient values of the graphs we may conclude that changes in nature property values are not affecting the ecotoxicity impact factor air, freshwater and agricultural soil emission world values. In all cases the value of R^2 is 1, represents the points are well fitted on the regression line, and only for fresh water ecotoxocity impact factor air emission World the regression line is slightly inclined toward Y-axis which is negligible.

On the other hand, for ecotoxicity impact factor air, freshwater and agricultural soil emission Europe an average slope 1.45 is observed, which represents a major influence on characterisation factors with the change in nature property values. Even in some cases, Fresh water ecotoxicity impact factor air emission Europe, the new CFs are two times greater compared to the old values for some substances, e.g., substance CAS number 80-62-6, 71-43-2 and 106-99-0 (see appendix)

4.2 Human damage factor

The human damage factor (HDF) in OMNIITOX base model describes the effect in cases for a species per kg emission (cases/kg). In the interpretation of the CFs BM distinguishes three different pathways: air, fresh water and agricultural soil emission as well as differentiates between cancer and non-cancer effects. Figure from 4.4 to 4.9 shows the HDF Europe and World for both cancer and non-cancer effects.

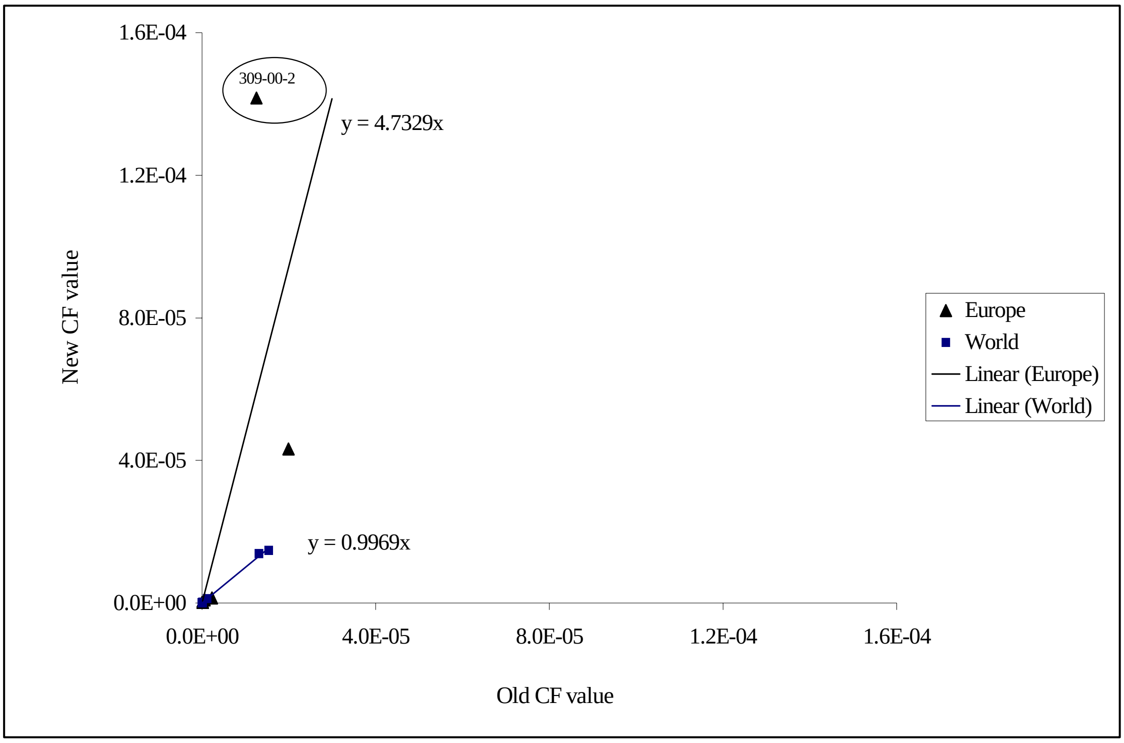

Figure 4.4: Human damage factor air emission Europe and World cancer effect.

For HDF World the comparison of old and new CFs respectively between cancer and non-cancer reveals an almost perfect correlation with a minor shifting in case of air emission. In most cases CFs are unchanged with the change in nature properties. This is probably due to a lack of nature property values, which can influence the HDF World values.

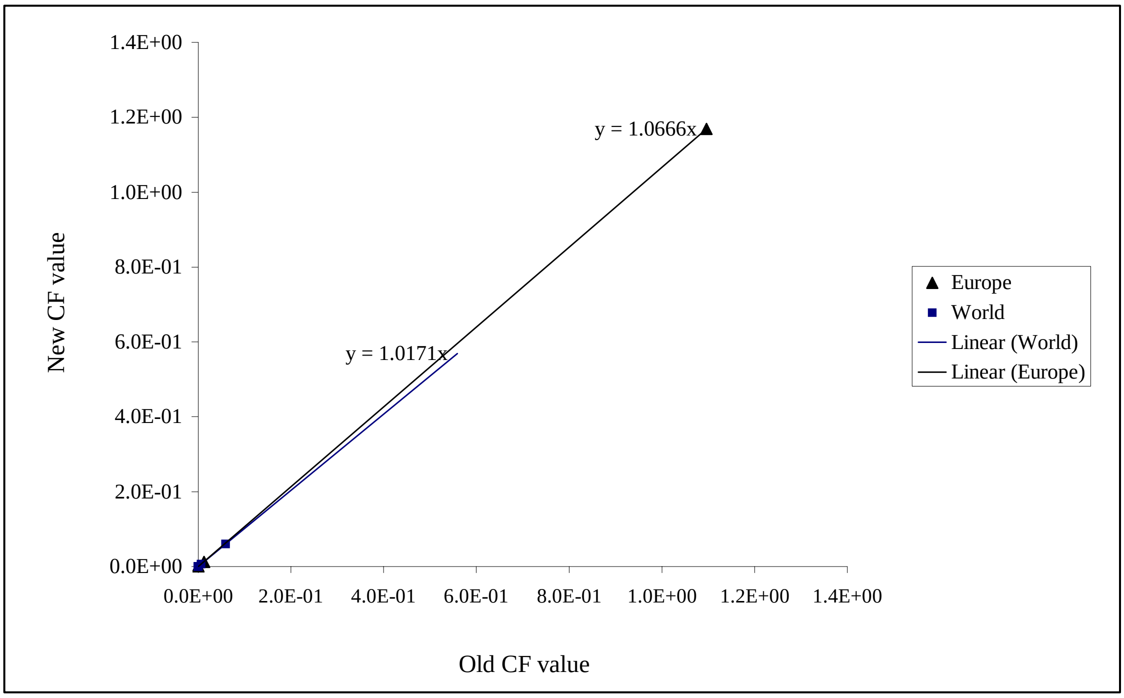

Figure 4.5: Human damage factor air emission Europe and World non-cancer effect.

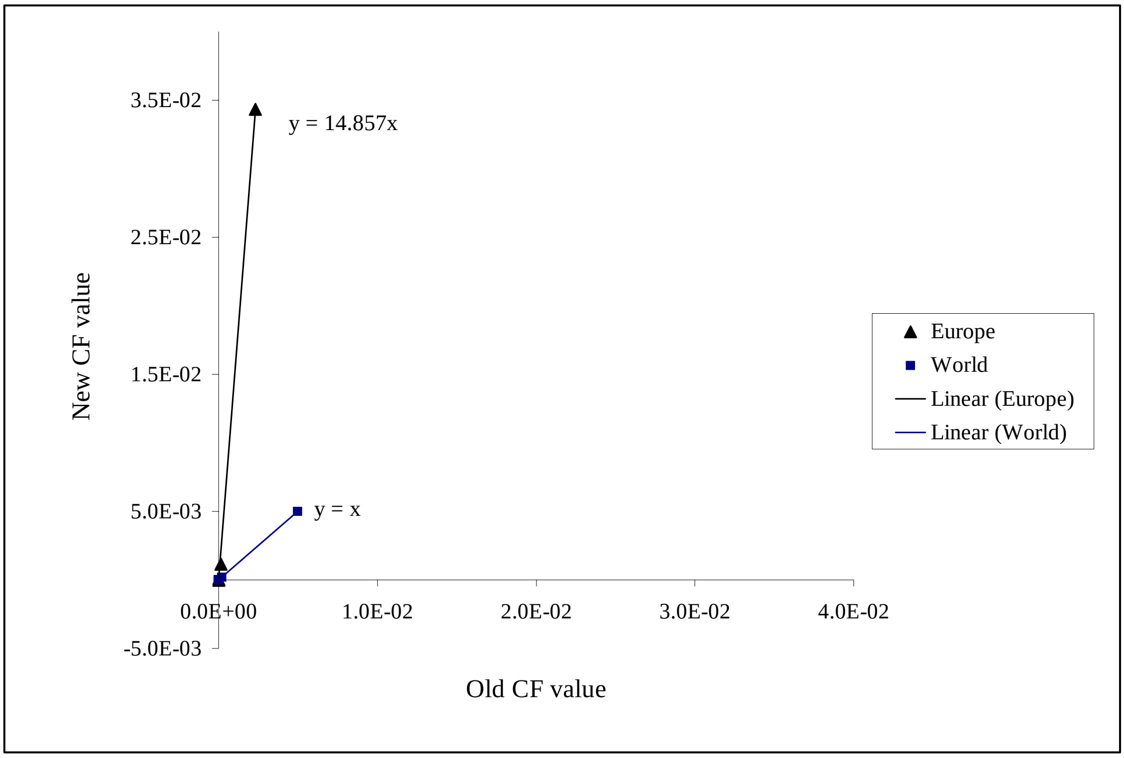

Figure 4.6: Human damage factor fresh water emission Europe and World cancer effect.

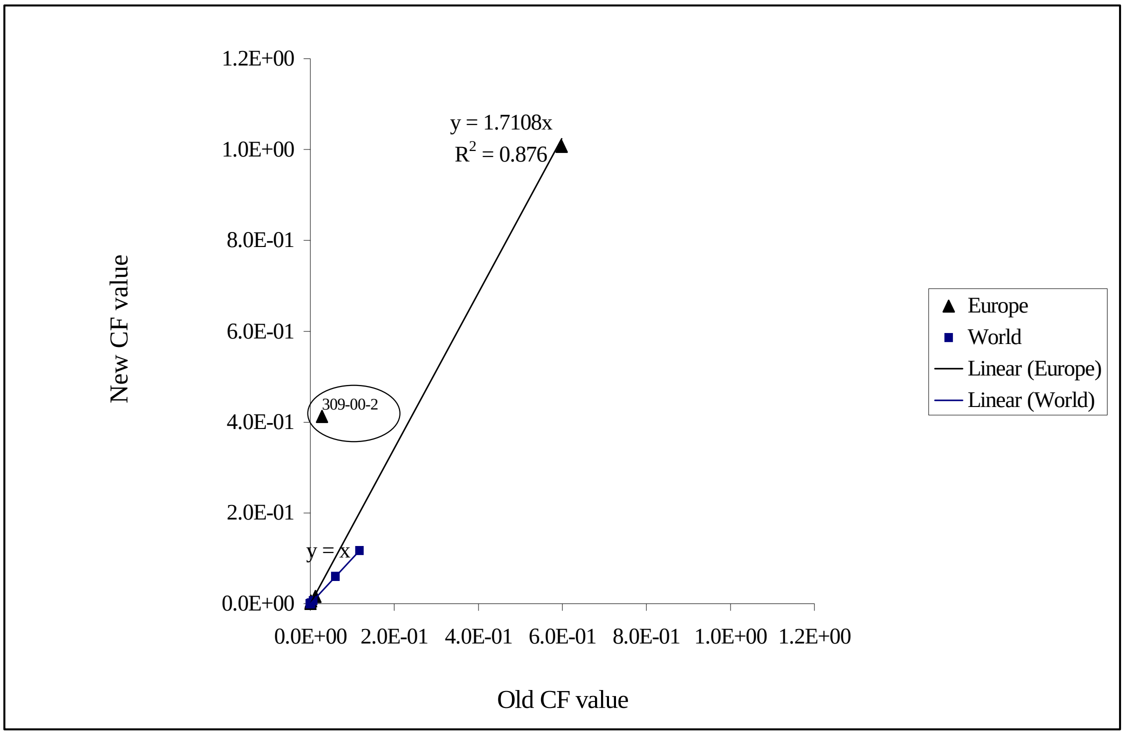

Figure 4.7: Human damage factor fresh water emission Europe and World non-cancer effect.

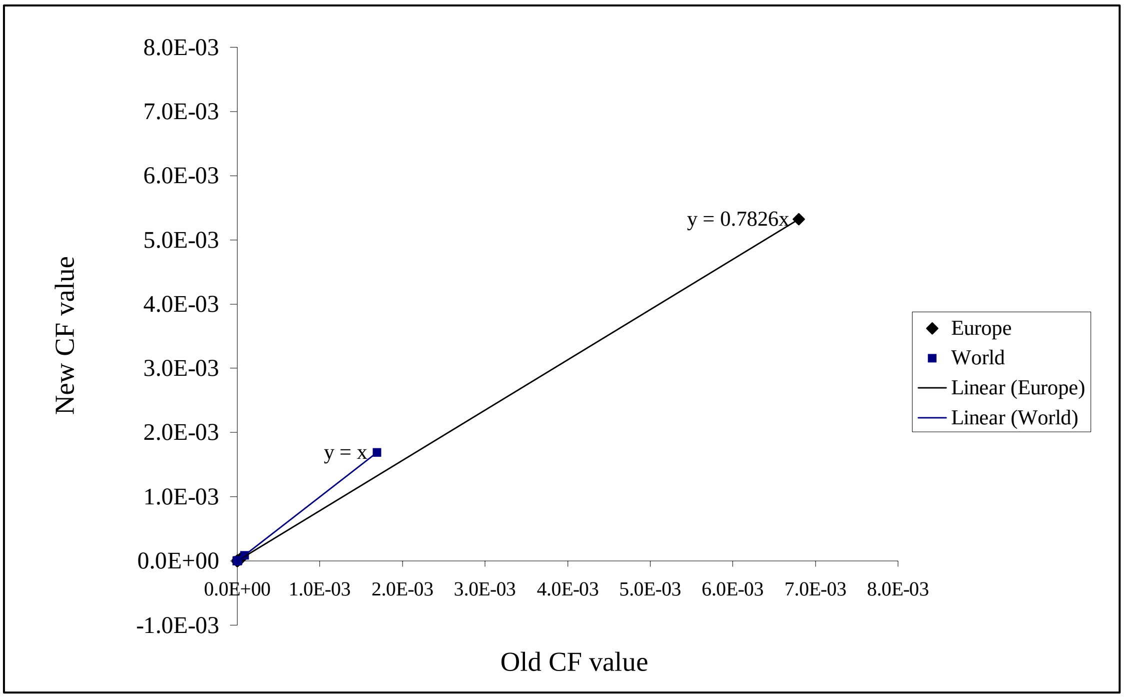

Figure 4.8: Human damage factor agricultural soil emission Europe and World cancer effect.

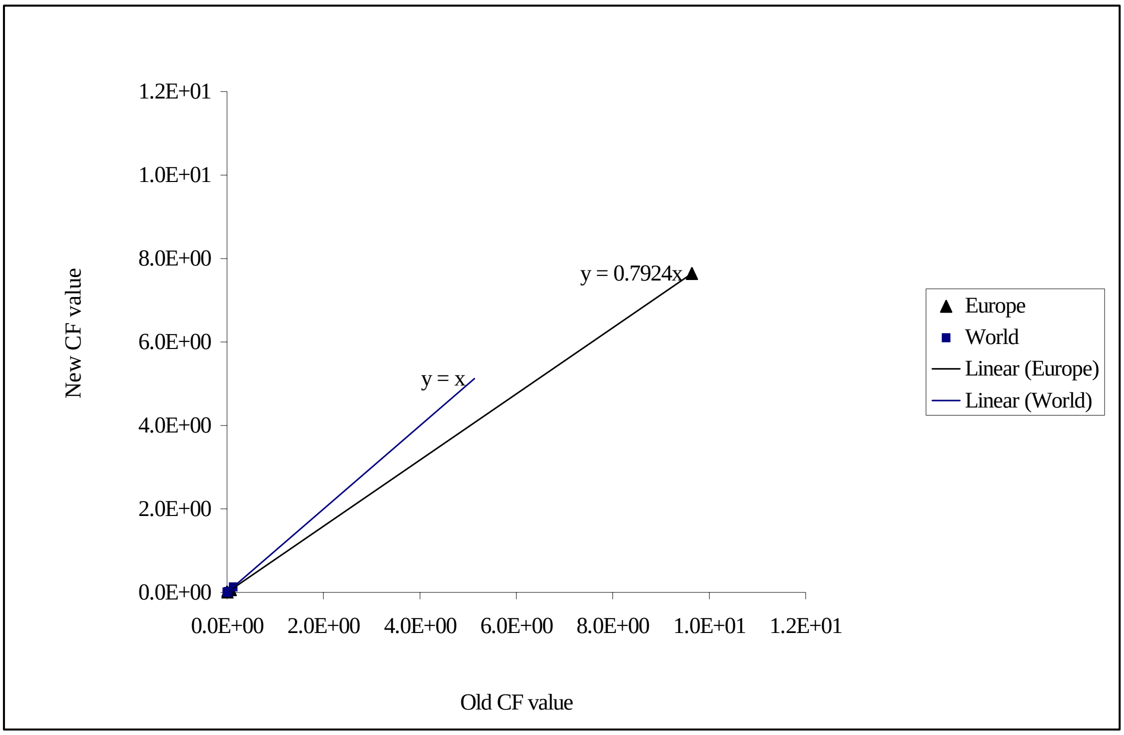

Figure 4.9: Human damage factor agricultural soil emission Europe and World non-cancer effect.

From the above figures we can see that the HDF air and soil emission Europe regression line shift toward Y-axis, i.e., CFs for new system boundary are dominating over old system boundary. The exception is HDF gricultural soil emission Europe both for cancer and non cancer effect, where the regression line shift toward the X-axis, i.e., old nature property values have greater effect on HDF agricultural soil emission Europe. In a number of cases the HDF values are deviating; marked in figure 4.4 and figure 4.7; from the regression line for few substances, e.g., substance CAS number 309-00-2, 87-68-3, 7440-43-9 are giving irregular values (see appendix).

The sensitivity analysis of OMNIITOX base model is dominated by several limitations. First of all, knowledge about the OMNIITOX model and related other multimedia models. To perform a sensitivity analysis it is very important to understand the model. In OMNIITOX documentaition nature framework properties are not well defined. Further specification of nature framework properties is necessary. Furthermore, it is difficult to understand how the calculation matrix is working in OMNIITOX IS to calculate the CFs.

Standardisation method for data gathering is also important to ensure the analysis method sophistication and to assess the data quality. In many cases the data sources do not document the data acquisition method. Aggregation of country level data is also a concern for some nature properties. In addition, very few substances give a very small population of CFs to analyse.

5. Conclusion

Increased focus on nature framework property, which is one of the essential parts of the OMNIITOX base model, has motivated this work. The need for sensitivity analysis, toward nature framework properties, is to define where the system potential changes. The different steps of the model sensitivity analysis have been described and the output has been evaluated.

The characterisaiton factors are influenced with the change in nature framework property values. It was assumed that the new system boundary would have an influence on characterisation factors as well as on nature framework property values. Implementing the new values in the OMNIITOX IS and comparing the outputs it may conclude that the OMNIITOX base model is sensitive toward nature framework properties.

The influence of the nature properties should be determined in order to understand why and when they are dominating. In fact this thesis can be a step toward further analysis of the OMNIITOX BM sensitivity to get more precise results of characterisation factors. Because in this work characterisation factors for only 19 substances were calculated which gave a very small population of data and is not sufficient for perfect regression analysis Further analysis is recommended implementing more substance and nature property values.

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7. Appendix

Table 1: Prioritised nature framework properties.

Mechanism parameter	**Unit**	**Value**	**Description**	**Category**
Area total Europe	m2	4.123E+12		Geographical
Area of soil compartment Europe	m2	3.08E+12		Geographical
Area of soil compartment World	m2	1.36E+14		Geographical
Duration of dry period	Day	3.111	Same for world and europe	Hydrological
Duration of wet period	Day	0.222	Same for world and europe	Hydrological
Fraction of soil area occupied by plants in Europe	Dimensionless	0.1		Geographical
Human person intake rate of beef	kg/(day*person)	5.2E-2	Same for world and europe	Biophysical
Human person intake rate of egg	kg/(day*person)	4.03E-2	Same for world and europe	Biophysical
Human person intake rate of fresh water	kg/(day*person)	1	Same for world and europe	Biophysical
Human person intake rate of fresh water fish	kg/(day*person)	7.12E-4	Same for world and europe	Biophysical
Human person intake rate of milk	kg/(day*person)	9.56E-1	Same for world and europe	Biophysical
Human person intake rate of pig	kg/(day*person)	1.4E-1	Same for world and europe	Biophysical

Mechanism parameter	**Unit**	**Value**	**Description**	**Category**
Human person intake rate of plant	kg/(day*person)	0.45	Same europe and world	Biophysical
Human person intake rate of poultry	kg/(day*person)	5.48E-2	Same for world and europe	Biophysical
Human person intake rate of sea water fish	kg/(day*person)	1.07E-2	Same for world and europe	Biophysical
Human person intake rate of sheep	kg/(day*person)	7.1E-3	Same for world and europe	Biophysical
Mean air flow Europe to World	m3/day	1.704E+15		Meteorological
Mean air flow to World Europe	m3/day	1.704E+15		Meteorological
Mean air temperature in Europe	K	281	NFP data	Meteorological
Mean depth of coastal sea water	m	0.03	Same for world and europe	Hydrological
Mean depth of fresh water in Europe	m	0.03	(Not same Europe and world)	Hydrological
Mean depth of soil compartment	m	0.3	Same for world and europe	Geological
Precipitation rate Europe	m/day	0.00208	“yearly rainfall” air module “rate of wet precipitation ” soil module	Hydrological
Production rate of harvest of plants in Europe	kg/day	1.27E+09		Biophysical

Mechanism parameter	Unit	Value	Description	Category
Production rate of irrigation water in Europe	m3/day	2.49E+08		Hydrological
Production rate of total bulk plants in Europe	kg/day	9.8E+09		Biophysical
Rate of ground water recharge	m/day	1.14E-5	Same for world and europe	Hydrological
Rate of runoff	m/day	5.83E-4	Same for world and europe 24 * 2.43*10E-5m/day	Hydrological
Surface area of fresh water compartment Europe	m2	1.08E11		Geographical
Surface area of sea water compartment Europe	m2	2.505E+12		Geographical
Total dry plant mass in Europe	kg	5.54E+12		Biophysical
Water flow from fresh water in Europe to fresh water in World	m3/day	1.60E-07		Hydrological
Water flow from fresh water in World to fresh water in Europe	m3/day	2.23E+05		Hydrological
Water flow from fresh water to sea water in Europe	m3/day	3.76E+07		Hydrological

Table 2: Fresh water ecotoxicity impact factor air emission Europe.

Substance CAS number	CFs for old NFP values	CFs for new NFP values
7440-47-3	1.188E+03	1.845E+03
7440-43-9	0.000E+00	0.000E+00
87-68-3	1.537E+00	1.975E+00
80-62-6	4.031E-05	8.541E-05
79-34-5	1.880E-02	2.447E-02
79-10-7	1.696E-03	2.556E-03
77-47-4	1.705E-01	2.272E-01
71-43-2	5.916E-04	1.265E-03
67-64-1	6.253E-06	8.794E-06
67-56-1	5.991E-06	8.598E-06
58-89-9	0.000E+00	0.000E+00
56-23-5	1.377E-02	1.772E-02
50-00-0	0.000E+00	0.000E+00
309-00-2	0.000E+00	0.000E+00
118-74-1	1.616E+01	2.026E+01
107-06-2	0.000E+00	0.000E+00
106-99-0	1.120E-04	2.640E-04
106-46-7	1.041E-01	1.430E-01
100-42-5	0.000E+00	0.000E+00

Table 3: Fresh water ecotoxicity impact factor air emission World

Substance CAS number	CFs for old NFP values	CFs for new NFP values
7440-47-3	3.690E+02	3.781E+02
7440-43-9	0.000E+00	0.000E+00
87-68-3	9.131E-01	9.277E-01
80-62-6	1.752E-05	1.767E-05
79-34-5	1.059E-02	1.075E-02
79-10-7	6.500E-04	6.509E-04
77-47-4	9.964E-02	1.013E-01
71-43-2	2.559E-04	2.582E-04
67-64-1	2.619E-06	2.633E-06
67-56-1	2.252E-06	2.254E-06
58-89-9	0.000E+00	0.000E+00
56-23-5	8.040E-03	8.173E-03
50-00-0	0.000E+00	0.000E+00
309-00-2	0.000E+00	0.000E+00
118-74-1	1.097E+01	1.110E+01
107-06-2	0.000E+00	0.000E+00
106-99-0	4.627E-05	4.643E-05
106-46-7	5.847E-02	5.948E-02
100-42-5	0.000E+00	0.000E+00

Table 4: Fresh water ecotoxicity impact factor fresh water emission Europe

Substance CAS number	CFs for old NFP values	CFs for new NFP values
7440-47-3	5.285E+03	7.456E+03
7440-43-9	0.000E+00	0.000E+00
87-68-3	1.955E+02	1.958E+02
80-62-6	3.508E-02	3.509E-02
79-34-5	2.439E+00	2.444E+00
79-10-7	2.758E-01	2.758E-01
77-47-4	2.496E+01	2.496E+01
71-43-2	5.724E-01	5.726E-01
67-64-1	9.042E-04	9.044E-04
67-56-1	8.578E-04	8.579E-04
58-89-9	0.000E+00	0.000E+00
56-23-5	1.749E+00	1.751E+00
50-00-0	0.000E+00	0.000E+00
309-00-2	0.000E+00	0.000E+00
118-74-1	1.659E+03	1.664E+03
107-06-2	0.000E+00	0.000E+00
106-99-0	3.317E-01	3.317E-01
106-46-7	1.604E+01	1.606E+01
100-42-5	0.000E+00	0.000E+00

Table 5: Fresh water ecotoxicity impact factor fresh water emission World.

Substance CAS number	CFs for old NFP values	CFs for new NFP values
7440-47-3	1.013E+03	1.013E+03
7440-43-9	0.000E+00	0.000E+00
87-68-3	1.941E+02	1.941E+02
80-62-6	3.507E-02	3.507E-02
79-34-5	2.424E+00	2.424E+00
79-10-7	2.757E-01	2.757E-01
77-47-4	2.494E+01	2.494E+01
71-43-2	5.718E-01	5.718E-01
67-64-1	9.040E-04	9.040E-04
67-56-1	8.576E-04	8.576E-04
58-89-9	0.000E+00	0.000E+00
56-23-5	1.737E+00	1.737E+00
50-00-0	0.000E+00	0.000E+00
309-00-2	0.000E+00	0.000E+00
118-74-1	1.634E+03	1.634E+03
107-06-2	0.000E+00	0.000E+00
106-99-0	3.313E-01	3.313E-01
106-46-7	1.593E+01	1.593E+01
100-42-5	0.000E+00	0.000E+00

Table 6: Fresh water ecotoxicity impact factor agricultural soil emission Europe.

Substance CAS number	CFs for old NFP values	CFs for new NFP values
7440-47-3	4.559E+03	6.431E+03
7440-43-9	0.000E+00	0.000E+00
87-68-3	1.769E-02	1.945E-02
80-62-6	1.104E-05	1.116E-05
79-34-5	4.032E-02	4.363E-02
79-10-7	3.783E-04	3.861E-04
77-47-4	5.238E-04	6.043E-04
71-43-2	2.936E-03	3.247E-03
67-64-1	3.195E-06	3.350E-06
67-56-1	1.893E-06	1.896E-06
58-89-9	0.000E+00	0.000E+00
56-23-5	1.486E-02	1.816E-02
50-00-0	0.000E+00	0.000E+00
309-00-2	0.000E+00	0.000E+00
118-74-1	3.408E+00	3.869E+00
107-06-2	0.000E+00	0.000E+00
106-99-0	3.631E-04	4.870E-04
106-46-7	4.107E-02	4.441E-02
100-42-5	0.000E+00	0.000E+00

Table 7: Fresh water ecotoxicity impact factor agricultural soil emission World.

Substance CAS number	CFs for old NFP values	CFs for new NFP values
7440-47-3	1.013E+03	1.013E+03
7440-43-9	0.000E+00	0.000E+00
87-68-3	5.286E+00	5.286E+00
80-62-6	1.059E-04	1.059E-04
79-34-5	1.666E-01	1.667E-01
79-10-7	7.052E-04	7.052E-04
77-47-4	1.713E-01	1.713E-01
71-43-2	5.158E-03	5.159E-03
67-64-1	3.456E-06	3.458E-06
67-56-1	2.855E-06	2.855E-06
58-89-9	0.000E+00	0.000E+00
56-23-5	3.549E-02	3.560E-02
50-00-0	0.000E+00	0.000E+00
309-00-2	0.000E+00	0.000E+00
118-74-1	7.295E+02	7.295E+02
107-06-2	0.000E+00	0.000E+00
106-99-0	7.308E-04	7.309E-04
106-46-7	1.187E+00	1.187E+00
100-42-5	0.000E+00	0.000E+00

Table 8: Human damage factor air emission Europe cancer effect.

Substance CAS number	CFs for old NFP values	CFs for new NFP values
7440-47-3	0.000E+00	0.000E+00
7440-43-9	2.229E-06	1.437E-06
87-68-3	7.995E-08	1.087E-07
80-62-6	0.000E+00	0.000E+00
79-34-5	1.883E-07	1.903E-07
79-10-7	0.000E+00	0.000E+00
77-47-4	0.000E+00	0.000E+00
71-43-2	9.511E-10	1.442E-09
67-64-1	0.000E+00	0.000E+00
67-56-1	0.000E+00	0.000E+00
58-89-9	5.596E-07	9.120E-07
56-23-5	1.579E-07	1.602E-07
50-00-0	2.422E-08	2.612E-08
309-00-2	1.255E-05	1.417E-04
118-74-1	1.988E-05	4.322E-05
107-06-2	9.962E-08	1.028E-07
106-99-0	7.641E-10	1.261E-09
106-46-7	6.624E-10	9.728E-10
100-42-5	0.000E+00	0.000E+00

Table 9: Human damage factor air emission Europe non-cancer effect.

Substance CAS number	CFs for old NFP values	CFs for new NFP values
7440-47-3	2.706E-06	3.060E-06
7440-43-9	1.096E+00	1.169E+00
87-68-3	4.178E-05	1.022E-04
80-62-6	5.395E-11	8.134E-11
79-34-5	1.794E-08	1.939E-08
79-10-7	1.042E-09	1.097E-09
77-47-4	7.744E-05	7.950E-05
71-43-2	8.858E-09	1.365E-08
67-64-1	4.286E-08	4.274E-08
67-56-1	1.434E-10	1.440E-10
58-89-9	2.677E-05	4.351E-05
56-23-5	2.046E-07	2.514E-07
50-00-0	2.507E-07	2.615E-07
309-00-2	1.429E-04	1.687E-03
118-74-1	1.264E-02	1.277E-02
107-06-2	1.118E-08	1.193E-08
106-99-0	1.189E-08	1.963E-08
106-46-7	1.026E-08	1.427E-08
100-42-5	3.528E-11	5.914E-11

Table 10: Human damage factor air emission World cancer effect.

Substance CAS number	CFs for old NFP values	CFs for new NFP values
7440-47-3	0.000E+00	0.000E+00
7440-43-9	1.213E-06	1.202E-06
87-68-3	4.562E-08	4.658E-08
80-62-6	0.000E+00	0.000E+00
79-34-5	9.431E-08	9.437E-08
79-10-7	0.000E+00	0.000E+00
77-47-4	0.000E+00	0.000E+00
71-43-2	3.627E-10	3.644E-10
67-64-1	0.000E+00	0.000E+00
67-56-1	0.000E+00	0.000E+00
58-89-9	1.650E-07	1.659E-07
56-23-5	8.510E-08	8.518E-08
50-00-0	6.267E-09	6.267E-09
309-00-2	1.540E-05	1.467E-05
118-74-1	1.314E-05	1.390E-05
107-06-2	4.919E-08	4.928E-08
106-99-0	2.794E-10	2.799E-10
106-46-7	2.890E-10	2.971E-10
100-42-5	0.000E+00	0.000E+00

Table 11: Human damage factor air emission World non-cancer effect.

Substance CAS number	CFs for old NFP values	CFs for new NFP values
7440-47-3	1.620E-07	1.670E-07
7440-43-9	5.908E-02	6.010E-02
87-68-3	2.758E-05	2.959E-05
80-62-6	1.953E-11	1.962E-11
79-34-5	7.568E-09	7.608E-09
79-10-7	3.294E-10	3.295E-10
77-47-4	4.132E-05	4.138E-05
71-43-2	3.209E-09	3.225E-09
67-64-1	1.569E-08	1.568E-08
67-56-1	4.538E-11	4.538E-11
58-89-9	7.899E-06	7.942E-06
56-23-5	1.030E-07	1.046E-07
50-00-0	8.029E-08	8.029E-08
309-00-2	1.717E-04	1.733E-04
118-74-1	6.372E-03	6.376E-03
107-06-2	4.842E-09	4.864E-09
106-99-0	4.336E-09	4.345E-09
106-46-7	4.612E-09	4.717E-09
100-42-5	1.271E-11	1.271E-11

Table 12: Human damage factor fresh water emission Europe cancer effect.

Substance CAS number	CFs for old NFP values	CFs for new NFP values
7440-47-3	0.000E+00	0.000E+00
7440-43-9	1.013E-20	-1.306E-20
87-68-3	9.702E-07	2.903E-06
80-62-6	0.000E+00	0.000E+00
79-34-5	8.379E-07	6.759E-07
79-10-7	0.000E+00	0.000E+00
77-47-4	0.000E+00	0.000E+00
71-43-2	1.652E-08	1.258E-08
67-64-1	0.000E+00	0.000E+00
67-56-1	0.000E+00	0.000E+00
58-89-9	8.682E-06	1.950E-05
56-23-5	9.960E-07	8.801E-07
50-00-0	1.636E-06	1.160E-06
309-00-2	2.307E-03	3.434E-02
118-74-1	1.459E-04	1.154E-03
107-06-2	3.151E-06	2.265E-06
106-99-0	1.208E-10	1.993E-10
106-46-7	4.384E-08	5.235E-08
100-42-5	0.000E+00	0.000E+00

Table 13: Human damage factor fresh water emission Europe non-cancer effect.

Substance CAS number	CFs for old NFP values	CFs for new NFP values
7440-47-3	9.828E-07	2.476E-06
7440-43-9	5.984E-01	1.007E+00
87-68-3	1.975E-03	6.039E-03
80-62-6	3.856E-09	2.837E-09
79-34-5	5.344E-07	4.184E-07
79-10-7	7.872E-09	5.631E-09
77-47-4	4.603E-06	6.491E-06
71-43-2	1.215E-06	9.183E-07
67-64-1	3.205E-08	2.294E-08
67-56-1	2.159E-09	1.572E-09
58-89-9	4.125E-04	9.262E-04
56-23-5	2.012E-05	1.756E-05
50-00-0	3.865E-08	2.754E-08
309-00-2	2.768E-02	4.120E-01
118-74-1	1.242E-02	1.611E-02
107-06-2	1.142E-06	8.168E-07
106-99-0	3.193E-07	2.368E-07
106-46-7	5.549E-07	6.624E-07
100-42-5	3.716E-09	3.393E-09

Table 14: Human damage factor fresh water emission World cancer effect.

Substance CAS number	CFs for old NFP values	CFs for new NFP values
7440-47-3	0.000E+00	0.000E+00
7440-43-9	5.448E-21	-2.023E-21
87-68-3	7.493E-07	7.498E-07
80-62-6	0.000E+00	0.000E+00
79-34-5	5.467E-07	5.467E-07
79-10-7	0.000E+00	0.000E+00
77-47-4	0.000E+00	0.000E+00
71-43-2	1.111E-08	1.111E-08
67-64-1	0.000E+00	0.000E+00
67-56-1	0.000E+00	0.000E+00
58-89-9	6.812E-06	6.812E-06
56-23-5	6.668E-07	6.669E-07
50-00-0	1.097E-06	1.097E-06
309-00-2	4.990E-03	4.990E-03
118-74-1	1.943E-04	1.950E-04
107-06-2	2.094E-06	2.095E-06
106-99-0	4.413E-11	4.421E-11
106-46-7	3.111E-08	3.111E-08
100-42-5	0.000E+00	0.000E+00

Table 15: Human damage factor fresh water emission World non-cancer effect.

Substance CAS number	CFs for old NFP values	CFs for new NFP values
7440-47-3	3.398E-07	3.398E-07
7440-43-9	1.169E-01	1.169E-01
87-68-3	1.540E-03	1.541E-03
80-62-6	2.595E-09	2.595E-09
79-34-5	3.578E-07	3.579E-07
79-10-7	5.282E-09	5.282E-09
77-47-4	2.665E-06	2.668E-06
71-43-2	8.192E-07	8.192E-07
67-64-1	2.090E-08	2.090E-08
67-56-1	1.451E-09	1.451E-09
58-89-9	3.236E-04	3.236E-04
56-23-5	1.373E-05	1.373E-05
50-00-0	2.576E-08	2.576E-08
309-00-2	5.987E-02	5.988E-02
118-74-1	6.681E-03	6.685E-03
107-06-2	7.616E-07	7.616E-07
106-99-0	2.142E-07	2.142E-07
106-46-7	3.935E-07	3.935E-07
100-42-5	2.559E-09	2.559E-09

Table 16: Human damage factor agricultural soil Europe emission cancer effect.

Substance CAS number	CFs for old NFP values	CFs for new NFP values
7440-47-3	0.000E+00	0.000E+00
7440-43-9	6.042E-21	-8.704E-21
87-68-3	3.109E-09	2.619E-09
80-62-6	0.000E+00	0.000E+00
79-34-5	2.180E-05	1.714E-05
79-10-7	0.000E+00	0.000E+00
77-47-4	0.000E+00	0.000E+00
71-43-2	2.379E-07	1.787E-07
67-64-1	0.000E+00	0.000E+00
67-56-1	0.000E+00	0.000E+00
58-89-9	3.555E-05	2.716E-05
56-23-5	5.810E-06	4.660E-06
50-00-0	1.390E-06	1.030E-06
309-00-2	6.800E-03	5.322E-03
118-74-1	5.187E-06	8.050E-06
107-06-2	4.103E-05	3.364E-05
106-99-0	6.098E-10	1.007E-09
106-46-7	6.099E-07	4.560E-07
100-42-5	0.000E+00	0.000E+00

Table 17: Human damage factor agricultural soil emission Europe non cancer effect.

Substance CAS number	CFs for old NFP values	CFs for new NFP values
7440-47-3	2.396E-05	1.959E-05
7440-43-9	9.640E+00	7.639E+00
87-68-3	6.017E-06	4.990E-06
80-62-6	2.927E-09	2.149E-09
79-34-5	1.557E-05	1.224E-05
79-10-7	1.228E-08	9.082E-09
77-47-4	1.142E-07	1.161E-07
71-43-2	1.760E-05	1.320E-05
67-64-1	3.249E-08	2.476E-08
67-56-1	1.114E-11	8.165E-12
58-89-9	1.688E-03	1.290E-03
56-23-5	1.260E-04	9.398E-05
50-00-0	4.149E-08	3.109E-08
309-00-2	7.366E-02	6.386E-02
118-74-1	1.429E-03	1.445E-03
107-06-2	1.506E-05	1.234E-05
106-99-0	7.352E-07	5.527E-07
106-46-7	7.704E-06	5.760E-06
100-42-5	4.231E-10	3.104E-10

Table 18: Human damage factor agricultural soil emission World cancer effect.

Substance CAS number	CFs for old NFP values	CFs for new NFP values
7440-47-3	0.000E+00	0.000E+00
7440-43-9	5.397E-21	-3.608E-21
87-68-3	2.098E-08	2.099E-08
80-62-6	0.000E+00	0.000E+00
79-34-5	3.430E-06	3.430E-06
79-10-7	0.000E+00	0.000E+00
77-47-4	0.000E+00	0.000E+00
71-43-2	3.917E-08	3.917E-08
67-64-1	0.000E+00	0.000E+00
67-56-1	0.000E+00	0.000E+00
58-89-9	6.013E-06	6.013E-06
56-23-5	1.009E-06	1.009E-06
50-00-0	2.292E-07	2.292E-07
309-00-2	1.692E-03	1.692E-03
118-74-1	8.763E-05	8.800E-05
107-06-2	6.811E-06	6.811E-06
106-99-0	2.219E-10	2.223E-10
106-46-7	9.476E-08	9.476E-08
100-42-5	0.000E+00	0.000E+00

Table 19: Human damage factor agricultural soil emission World non-cancer effect.

Substance CAS number	CFs for old NFP values	CFs for new NFP values
7440-47-3	3.426E-07	3.427E-07
7440-43-9	1.281E-01	1.281E-01
87-68-3	4.289E-05	4.292E-05
80-62-6	4.832E-10	4.832E-10
79-34-5	2.442E-06	2.442E-06
79-10-7	2.015E-09	2.015E-09
77-47-4	7.680E-08	7.690E-08
71-43-2	2.893E-06	2.893E-06
67-64-1	6.475E-09	6.475E-09
67-56-1	5.894E-12	5.894E-12
58-89-9	2.856E-04	2.856E-04
56-23-5	2.091E-05	2.091E-05
50-00-0	8.190E-09	8.190E-09
309-00-2	2.030E-02	2.030E-02
118-74-1	3.373E-03	3.375E-03
107-06-2	2.493E-06	2.493E-06
106-99-0	1.244E-07	1.244E-07
106-46-7	1.197E-06	1.197E-06
100-42-5	9.127E-11	9.127E-11