Life Cycle Impact Assessment of chemicals: relevance and feasibility of spatial differentiation for ecotoxicity and human toxicity impact assessment

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Abstract

Environmental implications of the whole supply-chain of products, both goods and services, their use, and waste management, i.e. their entire life cycle from “cradle to grave” have to be considered to achieve more sustainable production and consumption patterns. Historically, Life Cycle Management (LCM), Assessment (LCA) and the related Impact Assessment (LCIA) methods have mostly relied on site-generic, not spatially resolved, models. In recent years, the relevance of accounting for spatial differentiation has been increasingly discussed in the context of LCA. Thus, several spatially distributed fate and transport models of chemicals, i.e. models allowing spatially explicit assessment of contaminants from a given spatial distribution of emission, were developed. The present paper presents an overview of these models, and discusses the relevance and feasibility of spatial differentiation of LCIA results in a Life Cycle Management perspective. Example of application of the models for human and ecotoxicity impact categories at various scales are presented.

1 Introduction

Life Cycle Management (LCM) has been developed as a business approach for managing the total life cycle of products and services and as a framework to analyse and manage their sustainability performance. LCM is a business approach that goes beyond short-term success and aims at long-term value creation [1].

This approach requires companies to move away from just looking at their own operations and to look at what is happening in their value chain (upstream and downstream operations that are outside the company's direct control). One of the aims of LCM is to identify the potential environmental risks at each stage and Establish proactive systems to pursue the opportunities and manage or minimise the risks. Traditionally, the focus on improving production conditions has been at a local level. Today, as more products (goods and services) are traded regionally and globally, a geographical perspective on sustainability is utterly needed.

ISO 14044:2006 foresees that "Depending on the environmental mechanism and the goal and scope, spatial and temporal differentiation of the characterization model relating the LCI results to the category indicator should be considered." Actually, there is a lack of spatially or temporally differentiated LCI data and corresponding LCIA methods. Hence, for the time being such differentiation is in practice not or rarely feasible [2].

As attention to chemical's impact grows, product life cycle management is becoming a crucial issue in realizing a sustainable society. In this context, one of the main goals is to provide decision support at policy and corporate level necessary for understanding the behaviour and fate of chemical along the life cycle of a product while minimizing potential impact.

So far, life cycle impact assessment (LCIA) methods have mostly relied on generic or non-spatial multimedia environmental models. There is continual debate whether the exclusion of spatial information in applications such as Life Cycle Assessment (LCA) may lead to misleading results, influencing the decision on products environmental performance.

Actually, distribution and fate of chemicals in the environment present an high variability depending on geographical location.

Spatial differentiation is recognized to be a timely and relevant issue to be addressed in order to reduce uncertainties. Taking the example of human toxicity and ecotoxicity impact categories, in recent years, several spatially distributed fate and transport models of chemicals, i.e. models allowing spatially explicit representations of contaminants from a given spatial distribution of emission, were developed (such as [3] and [4]).

Despite this underlying research work, practical recommendations how to reduce uncertainty and improve the relevance of LCA results by addressing spatial differentiation have still not been implemented in the daily LCA practice. Moreover, asking an LCA practitioner to address spatial differentiation has important drawbacks in term of workload (e.g. input data to be provided) and computational capacities.

This study, is part of the European project LC-IMPACT, and aims at discussing the relevance of spatial differentiation of chemicals emissions in order to support life cycle management.

To do so, we present an overview of multimedia models, identifying the critical aspects and discussing the role of geographical differentiation.

More specifically, we evaluate the spatial variability of the environmental concentration and characterization factors at a country, continental and global scale using three distinct multimedia models MAPPE Europe [5], IMPACT World [6], and USEtox [7]. Having a different level of spatial resolution, these models, support the assessment of conditions/emission scenarios which warrant spatial resolution for characterisation factors concerning ecotoxicity and human toxicity. As a first step, guidance on spatial distribution can be based only on physical-chemical properties and may support the identification of the range/distribution of the chemical (from local to global scale) [8]. However, it is necessary to run multimedia models in order to perform a comprehensive analysis of spatial variability. This represents a fundamental step for further identification of appropriate archetypes as a simplified approach to spatial modelling.

2 Overview of models suitable for spatial differentiation of chemical's impact

In the context of chemical impact assessment an assessment of some key existing models were undertaken in order to assess whether spatial differentiation is needed, and in which cases taking into account geographical variability is crucial. The overview methods and model able to calculate spatially differentiated characterisation factors was carried out also in light of balancing the uncertainties related to site-independent models and the complexity/workload of those that are site-dependent.

The main criteria for assessing strength and weakness of the selected models were focused on:

- Environmental compartment/media modelled and considered
- Accounting for transboundary transport
- Exposure pathways considered
- Capability of identifying hot spots (high exposure intensity)
- Geographical coverage
- Model's resolution

Tab.1: Synoptic scheme of the main model type for assessing spatial differentiation in the context of Life Cycle Impact Assessment (modified from [5]).

Model type	Model name	Multiple Environmental Media	Transboundary transport	Multi-pathway exposure	High exposure intensity	Global coverage
Generic/ nested Multimedia	CALTox [9]	one-box	One-box	Ingestion/ inhalation/ dermal	-	no
	USETox [6]	Urban/cont/global	Water and air advection	Ingestion/ Inhalation	Urban compartment	Global
	USES-LCA [3]	Local/region/ cont/hemispheric	Water and air advection	Ingestion/ Inhalation	Local environment.	Hemispheric
Spatial Multimedia	IMPACTEurope [10] and NorthAmerica [11]	136 watersh./ 157aircells 523 watersh./	Water and air advection	Ingestion/ Inhalation	Urban compartment/ + watershed agr.Product	Europe /North America
	GLOBOX [3]	239 countries	Water and air advection	Ingestion/ Inhalation	country	Global
	IMPACTWorld [5]	17 sub-cont. regions 9 oceans + 33 coastal regions	Water & air advection and food trade	Ingestion/ Inhalation	Urban compartment/ costal area	Global
	Mappe Europe [4]	1x1 km	Source-receptor matrix	-	Local condition	Europe
	Mappe Global [12]	1x1 degree	Advection from cell accounted	-	Local condition	Global
Global Climate + Atmospheric transport.	GEOS-Chem [13]	Air 2x2.5 degree air cells	-	-	-	Global

In Table 1, a synoptic overview of the typology of models (with few key examples) for assessing spatial differentiation in the context of Life Cycle Impact Assessment is presented. In the table is also showed the extent to which different types of models (generic/nested multimedia, spatial multimedia and global multimedia) meet the key criteria described above.

Multimedia models like USEtox [7] simulate pollutant transport through air, water and soil, with the one-box version (or a nested box) using averaged environmental and exposure parameters to estimate concentrations and intake fractions, roughly estimating impacts in the emission region. Anyway, they cannot account for spatial differentiation.

Impact 2002+ Europe [10] and North America [11] and MAPPE Europe [5] are able to predict monitored concentration but the geographical coverage cannot cover the entire world. Nevertheless, MAPPE Europe is highly spatially resolved and provides a user-friendly way to simulate fluxes and concentrations of chemical pollutants at a resolution of 1x1 Km in Europe.

MAPPE Global [12] is a spatially-resolved steady state multimedia model capable to calculate removal rate at a resolution of 1x1 degree for the entire globe but lack of a fully integrated atmospheric transport model.

The recent development of the GLOBOX model [4] represents the first global multimedia model to include exposure. The model could calculate spatially differentiated LCA toxicity characterisation factors on a global scale. It builds upon EUSES 2.0 multimedia model, supplemented by specific equation to account for advection of air and water. However, it does not account for urban exposure and it has not yet been compared with or evaluated against measurements and some limitation related to pollutant transport between regions were identified [6].

IMPACT World [6] enables to determine Intake Fractions (iF) and characterization factors (CF) for 17 regions of the world, differentiating between location of emission and location of impact.

Therefore, none of the above models fully meet the criteria required for evaluating the globally-distributed human toxicity and ecotoxicity impacts associated to pollutant emissions.

To assess how to further develop suitable models and to identify archetypes of emission to simplify the spatial differentiation, three models were run.

In the following section, example of the results, IMPACT World and Mappe Europe are provided.

3 Results

Examples of results from different models are presented in the following sections, covering various resolutions and chemicals to highlight extent of spatial variability.

3.1 IMPACT World

IMPACT World [6] divides the world into 17 sub-continental regions, 9 ocean regions, and 33 coastal regions As in previous IMPACT versions [10], each continental region consists of an air zone (containing an air compartment) and a terrestrial zone (containing water, soil, vegetation, roots, and sediment), and each ocean region consists of an air zone and an ocean zone (containing surface ocean, deep ocean, and ocean sediment).

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. The model accuracy was increased while minimizing complexity by embedding a regionally-parameterized urban box to account for urban emissions and exposure in each region.

Trans-boundary pollutant transport can occur between regions through water flows and, more importantly for the applications considered here, air flows. The regional divisions are based on a combination of geography (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). Due to river runoff and high coastal population density, much of the ocean pollution is concentrated in coastal areas, which are relatively shallow and contain up to 90% of the global fisheries catch [14]. GIS were used to define coastal regions as the sections of ocean adjacent to land that are less than 150 m in depth, which includes most of the continental shelf [15].

A multipartitioning chemical (Lindane) was chosen to run the model. For multipartitioning chemicals it is expected that removal rates and fate compartments change more according to environmental parameters than other kind of chemicals. Furthermore, the high persistence of Lindane (banned in many countries as a POP) represent a reference chemical for modelling impact that may occur far from the source of emission.

An example related to the intake fraction due to ingestion calculated with IMPACT World is presented in Fig. 1.

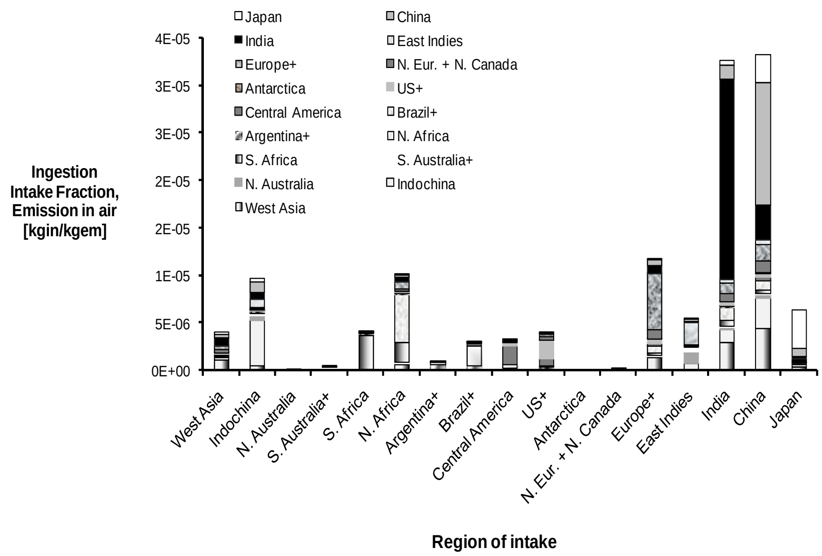

Fig.1: Intake fraction of Lindane due to ingestion. In the plot, each bar corresponds to the overall intake fraction due to an emission in a certain area and the contribution to the result due to each region of the intake.

Fig.1 shows that the oral intake fraction varies greatly from region to region i.e., China has a global intake factor 36 higher than in Argentina (3.32E-5 vs. 9.23E-7 kgin/kgemit, respectively). Breaking this down by region of intake, 64% of the intake fraction from an India emission is ingested locally (i.e., intake in the region of emission). Even though local intake dominates most intake fractions (iFs), transboundary transport accounts for more than 65% of the intake due to emissions in the West Asia and N. Europe and N. Canada regions. Note that Chinese takes in more Indian emissions than vice-versa due to the dominating westerly winds.

3.2 Mappe Europe

In order to understand the spatial variability of chemicals distribution and fate, there is the need of testing models also at higher resolution. For this purpose, we run the multimedia model MAPPE Europe. This is a GIS based model which provides a user-friendly way to simulate fluxes and concentrations of chemical pollutants emitted by industrial activities, other chemical emission diffusive or point sources, or widespread used substances within households or urban environment. The target contaminants are organic compounds such as Persistent Organic Pollutants (e.g. polychlorinated biphenyls, dioxins), pesticides, pharmaceuticals, volatile organic compounds, or other industrial chemicals. Spatial extent is the European continent with resolution of 1x1 km. Using MAPPE Europe calculates annual average environmental concentration in air, soil, surface water and European seas as a basis for calculating spatially resolved characterisation factors.

The scenario for running the model was related to an industrial emission.

An emission of 1,1,1,2 tetrachloroethane was chosen to run the model considering a scenario of atmospheric emissions from industrialized (urban) areas in Europe. 1,1,1,2 tetrachloroethane has the highest solvent power of any chlorinated hydrocarbon and once it was widely used as a solvent and as an intermediate in the industrial production of trichloroethylene, tetrachloroethylene, and 1,2-dichloroethylene.

The scenario assumes an overall amount of 100 tons emitted to air per year; latter was scaling by country on the basis of population density. Thus, the emissions from the smaller European countries (like Estonia or Slovenia) are in a range 0.1-1 t/y, while the industrial states (as Germany, UK France and Italy) emitted more then 10t/y (besides, Spain and Poland are also close to this amount emitting 7-8 t/y); for the other cases the emissions vary between 1-4 t/y.

Two maps of the results for 1,1,1,2 tetrachloroethane are reported in Fig.2 and 3.

In Fig.2, the higher concentrations in atmosphere are related to the source of emissions (populated areas under the considered scenario) but also to climatic conditions (for instance, even higher emissions in Spain or Italy, the elevated air removal rate leads to relatively lower concentrations in the southern compared to those in the central part of Europe).

In Fig.3, the spatial variability of 1,1,1,2-tetrachloroethane mass in soil after an emission in air is presented. In this case, the concentrations follow the pattern of the atmospheric deposition which explains why higher concentrations are predicted in the mountain areas, in which typically comparatively lower temperatures are expected.

Differences up to one order of magnitude, have been found under the 1,1,1,2-tetrachloroethane scenario described above, when comparing estimates of environmental concentrations (median or mean for Europe) produced by the highly resolute MAPPE with non-spatial USEtox model [8]. Generally, USEtox tends to overestimate the forecasts of MAPPE model and predicts values close to the upper bound (95% quantile) of MAPPE results.

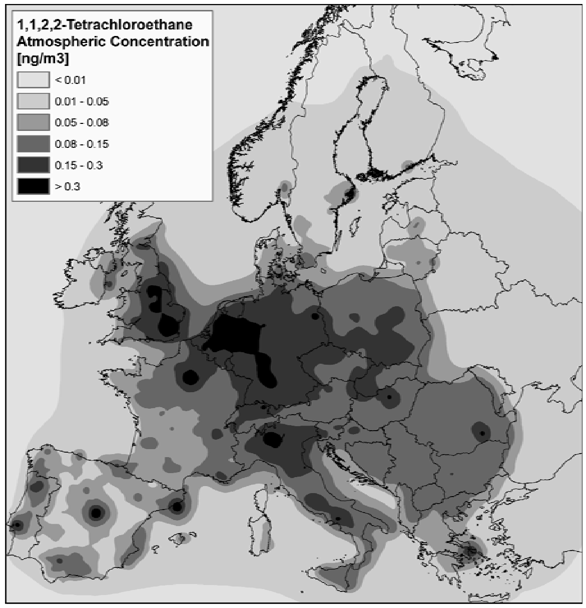

Fig.2: Concentration of 1,1,1,2 tetrachloroethane in air after an emission in air from highly industrialized areas

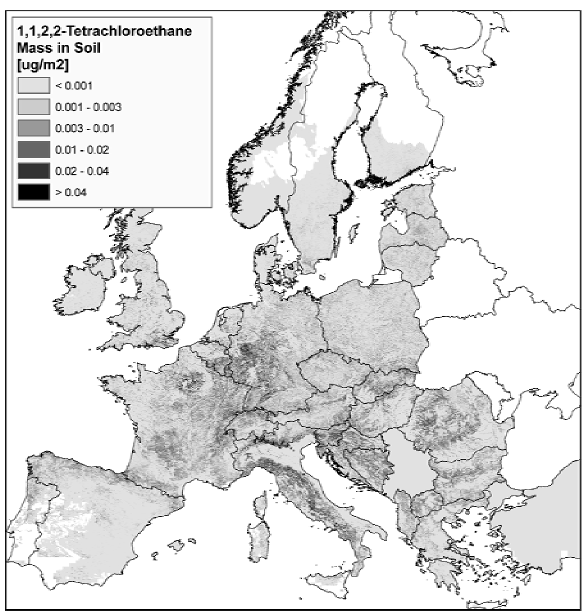

Fig.2: Concentration of 1,1,1,2 tetrachloroethane in soil after an emission in air

4 Discussion, implication for LCM and outlook

The examples presented above shows at which extent spatial variability may imply differences in the impact, depending on location of emission and on the specific scenario under assessment. Actually, even if the relevance of geographical differentiation for human and ecotoxicity is recognised as relevant, there is a lack of models able to perform a complete assessment of spatial differentiation

Some promising models with potential for application in the context of LCIA lack algorithms or proposals on how to calculate spatially resolved characterisation factors. Even if the models are scientifically robust a straightforward integration in the LCIA is not feasible and further development is needed.

Furthermore, the most feasible and meaningful degree of spatial differentiation is still to be determined in LCIA context, i.e. whether to divide by national boundaries (countries), natural geographical units or sub-units (continents and landscape zones), sub-compartments of the environment (e.g. different types of water bodies), emission situations (e.g. in areas with high or low human population density), or by geographical coordinates via a global impact grid, etc. This will need to be closely coordinated with data availability especially in industry, LCI modelling needs, review questions, and software and database management implications [2].

It is worthily to note that many issues are still under discussion in order to foster the robustness and acceptability of existing and new methods for spatial differentiation. Amongst the other, the following issues are upmost relevant:

- How to address uncertainties
- How to build archetypes of emission-receptor situations which support differentiation and calculate characterization factors to represent the archetypes
- How to calculate characterization factors per region and simplified equations enabling the practitioner to customize results to own cases
- How an in which case temporal aspects may change the final result (seasonality but also short-term/long term emission)
- How to support the collection of spatially resolved data at the inventory side

Nevertheless, spatially differentiation may play a relevant role in decision support in the context of Life Cycle Management.

Recently, in the ILCD recommendation for LCIA, a criteria for choosing most suitable methods for impact assessment, stated that as far as available, global models have to be used – also for regional impacts. In absence of sufficiently sound global models, a choice had to be made in favour of models that represent large heterogeneous regions qualifying them as proxies of a global situation [16]. The further development and provision of guidance on spatial differentiation will help practitioners to identify situations for which spatial differentiation in the life cycle impact assessment should be deemed relevant as well as how to create consistency between inventory and impact assessment regarding regionalization.

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6 References

[1] UNEP/SETAC. "Life Cycle Management: How business uses it to decrease footprint, create opportunities and make value chains more sustainable" report, 2009, pp.48

[2] European Commission - Joint Research Centre - Institute for Environment and Sustainability: International Reference Life Cycle Data System (ILCD) Handbook - General guide for Life Cycle Assessment - Detailed guidance. EUR 24708 EN. Luxembourg. Publications Office of the European Union; 2010 pp 417

[3] Macleod M., Riley W. J., McKone T. E., Assessing the influence of climate variability on atmospheric concentrations of polychlorinated biphenyls using a global-scale mass balance model (BETR-global). *Environmental Science and Technology*, 39, 2005, 6749-6756.

[4] Wegener Sleeswijk A, Heijungs R, GLOBOX: A spatially differentiated global fate, intake and effect model for toxicity assessment in LCA, *Science of the Total Environment*, 408,2010, pp.2817-2832

[5] Pistocchi A., Zulian G., Vizcaino P., Marinov D., Multimedia Assessment of Pollutant Pathways in the Environment, European scale model (MAPPE-EUROPE), Office for Official Publications of the European Communities, Luxembourg, EUR 24256 EN, DOI 10.2788/63765, 2010, 53p

[6] Shaked S., Multi-Continental Multimedia Model of Pollutant Intake and Application to Impacts of Global Emissions and Globally Traded Goods. PhD dissertation of the University of Michigan. 2011

[7] Rosenbaum R.K., Bachmann T.M., Gold L.S., Huijbregts M.A.J., Jolliet O., Juraske R., Koehler A., Larsen H.F., MacLeod M., Margni M., McKone T.E., Payet J., Schumacher M., van de Meent D., Hauschild M.Z., USEtox-the UNEP-SETAC toxicity model: recommended characterisation factors for human toxicity and freshwater ecotoxicity in life cycle impact assessment. *International Journal of Life Cycle Assessment* 13, 2008, pp. 532-546.

[8] Sala S, Marinov D., Pennington D. Spatial differentiation of chemical removal rates in Life Cycle Impact Assessment, *International Journal of Life Cycle Assessment* (submitted)

[9] Maddalena R.L., McKone T.E., Layton D.W., Hsieh D.P.H., Comparison of Multimedia transport and transformation models- regional fugacity models vs CALTox. *Chemosphere* 30, 1995, pp869-889.

[10] Pennington DW, Margni M, Ammann C, Jolliet O, Multimedia fate and human intake modelling: Spatial versus non spatial insights for chemical emissions in Western Europe, *Environmental Science and Technology*, Vol. 39, N 4, 2005, pp.1119-1128.

[11] Humbert S., Manneh R., Shaked S., Wannaz C., Horvath A., Deschenes L., Jolliet O., Margni M., Assessing regional intake fractions in North America. *Science of the Total Environment*, 407, 2009, pp.4812-4820.

[12] Pistocchi A, Marinov D, Pontes S, Zulian G, Multimedia assessment of pollutant pathways in the environment - Global scale model (MAPPE Global). 2011. EU Report (in preparation)

[13] Bey I., Jacob D.J., Yantosca R.M., Logan J.A., Field B.D., Fiore A.M., Li Q.B., Liu H.G.Y., Mickley L.J., Schultz M.G., Global modeling of tropospheric chemistry with assimilated meteorology: Model description and evaluation. *Journal of Geophysical Research- Atmospheres*, 106, 2001, pp. 23073-23095.

[14] Schwartz M.L., *Encyclopaedia of costal science*, Springer, Dordrecht, 2005.

[15] Chaudhary M., Chaudhary G., *Global encyclopaedia of political geography*, Global Vision Pub. House, 2009.

[16] EC- JRC, Recommendations based on existing environmental impact assessment models and factors for Life Cycle Assessment in European context. (In preparation) Draft available at http://lct.jrc.ec.europa.eu