LCIA OF IMPACTS ON HUMAN HEALTH AND ECOSYSTEMS (USEtox)

Assessing freshwater ecotoxicity of agricultural products in life cycle assessment (LCA): a case study of wheat using French agricultural practices databases and USEtox model

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Received: 30 December 2010 / Accepted: 28 June 2011 / Published online: 22 July 2011 $©$ Springer-Verlag 2011

Abstract

Purpose A life cycle assessment (LCA) was conducted on winter wheat, based on real agricultural practices databases, on a sample divided into four production scenarios. The main objectives of this study are (1) to assess the environmental impact of winter wheat, using an LCA covering field practices, and the transport and storage of grain until it is sold to a miller; (2) to use the USEtox model (Rosenbaum et al. in Int J Life Cycle Assess 13:532–546, [2008\)](#page-6-0) to assess the part of the total freshwater ecotoxicity impact due to pesticide use, its variability among plots, and to identify the active ingredients with the strongest impact; (3) and with the help of fungicide, insecticide, herbicide experts, to identify active ingredients to replace these highimpact pesticides and estimate the effect of such a substitution on total freshwater ecotoxicity.

Materials and methods InVivo (the authors' company) is a French union of agricultural cooperatives that produces and sells, amongst other products and services, decision-making tools to help farmers manage fertilization and pesticide applications. With the help of cooperatives and with the help of these tools, pedologic, climatologic and agronomic (in particular for fertilization and pesticide applications practices) data can be collected for each agricultural plot of a farm.

Results and discussion The main conclusions of this study are that : (1) when considering freshwater ecotoxicity impacts, pesticide use is predominant on the whole life

Responsible editor: Andreas Jørgensen

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cycle of winter wheat, (2) there is a huge scattering of the results observed between fields when compared to the low scattering of the results between the four production scenarios, (3) it is feasible, with the USEtox model, to identify the active ingredients with the strongest impact and to potentially decrease this average impact by 50% by substituting only three active ingredients.

Conclusions A further step to improve ecotoxicity assessment in LCAwould be to develop a model to better estimate the pesticide emissions pattern on field, taking into account pedo-climatic conditions and farmers' practices.

Keywords Agricultural production . Freshwater ecotoxicity. Life cycle assessment . Plant protection . Substitution active ingredient . USEtox . Wheat

1 Introduction

Life cycle assessment (LCA) is the leading methodology for environmental impacts assessment of a product for two principal reasons: it allows the calculation of several indicators corresponding to different environmental impacts (global warming, eutrophication, primary resources depletion…), and takes into account all relevant steps of the life cycle of a product, from the production of raw materials to the end of life.

Most of LCA of crop production focus on nitrate emissions (Brentrup et al. [2000](#page-6-0), [2002\)](#page-6-0) or greenhouse gases emissions (Biswas et al. [2007;](#page-6-0) Brentrup et al. [2002\)](#page-6-0). Pesticides and their effects on the ecosystems are still too often omitted in these studies even though they are one of the major environmental issues linked with agriculture. In France, in 2007, the monitoring of rivers and groundwater showed that 91% of the sampling sites for surface water

and 59% of the sampling points for groundwater showed a presence of pesticides (Dubois et al. [2010](#page-6-0)). The pesticide contents are often very low, but these results show the great scattering of pesticides in freshwater. A precise assessment of the effects of pesticides is then an important issue in an agricultural LCA.

Nevertheless, the use of pesticides in agriculture is essential with regard to food self-sufficiency and the staunch control of plant diseases. The good practice of agriculture is to apply the right pesticide only if necessary, at the right dose and at the right moment. In order to achieve this, farmers can be helped with specific tools.

Some studies have already worked on pesticide-induced ecotoxicity (Humbert et al. [2007](#page-6-0); Margni et al. [2001\)](#page-6-0) and were confronted with several challenges that constitute the main reasons why toxicity factors are not always tackled in LCA:

- Obtaining real data on agricultural practices, especially fertilization and pesticides applications (type of pesticides, doses, application technique, date of application…)
- Assessing the impact of these real practices using reliable and recognized models allowing the calculation of (1) the fractions of the applied pesticide emitted in the different compartments: air, water, soil and (2) the effect of these emissions on the environment.

Several methodologies concerning fate, exposure and effects of ecotoxic substances have been published: IMPACT 2002 (Jolliet et al. [2003\)](#page-6-0), USESLCA (Huijbregts et al. [2000](#page-6-0)), Eco-Indicator 99 (Goedkoop and Spriensma [2001\)](#page-6-0) and CalTOX (McKone and Enoch [2002\)](#page-6-0). In 2004, within the framework of the EU project OMNITOX, Pant et al. [\(2004](#page-6-0)) revealed that chemical emissions models commonly used in LCA vary to a significant extent in their modelling principles, thus in the characterization factors they produce. It motivated several representatives for models from Europe, North America and Asia to work on a survey of existing characterization models, proceeding to develop a "consensus model": USEtox (Hauschild et al. [2008\)](#page-6-0). This model comparison process allowed to identify differences between the models' results and structure, in order to then identify essential model components and to build a consensus model. A chemical test set of 45 chemicals, with different property combinations, was used to compare the models. A focus was done on the results concerning key fate, exposure and effect issues for the comparison (Rosenbaum et al. [2008](#page-6-0)).

The USEtox model tackles the estimation of characterization factors of chemicals emissions in different compartments, with regard to human toxicity and freshwater ecotoxicity. It contains a chemical fate model that takes into consideration a part of the substances' future in air, water and soil (Rosenbaum et al. [2008](#page-6-0)). However, the fate of the pesticide just after the application is not considered and need to be completed. The method of Audsley et al. ([2003](#page-5-0)) and the European Monitoring and Evaluation Programme (EMEP)–CORe INventory of AIR emissions (CORINAIR) method EMEP/EEA et al. ([2009\)](#page-6-0) enabled us to handle this aspect of the model. The other available models estimating these fate factors require many specific datasets that were not accessible for this study.

The main objectives of this study are (1) to assess the environmental impact of winter wheat, using an LCA covering the field practices, the transport and the storage of the grains, until the grain is sold to a miller, (2) to assess the part of the total freshwater ecotoxicity impact due to pesticide use, its variability among plots and to identify the most impacting active ingredients, (3) with the help of fungicide, insecticide, herbicide experts, to identify replacement active ingredients for these high-impact pesticides and to estimate the effect of such a substitution on total freshwater ecotoxicity.

2 Materials and methods

InVivo (the authors' company) is a French union of agricultural cooperatives that produces and sells, amongst other products and services, decision-making tools to help farmers manage fertilization and pesticide applications. With the help of cooperatives and with the help of these tools, pedologic, climatologic and agronomic (in particular for fertilization and pesticide applications practices) data can be collected for each agricultural plot of a farm.

2.1 Data collection

An LCA was conducted on winter wheat, based on real agricultural practices recorded for winter wheat harvested in 2009, on a sample of 6,679 plots, covering 44,494 ha in the north east of France. The real agricultural practices were directly recorded with a tool used by farmers to manage their practices and to permit traceability of their products. To use this tool, farmers had to record all their field operations. Through this decision-making tool, data on pedology and agricultural practices for each plot in which this tool is used were gathered in a database and were analysed using the software Statistic Analysis System (SAS 9.2 [2008\)](#page-6-0). Thus, the results of this LCA are representative of farmers who are using decision-making tools.

The plots were divided into four groups, corresponding to four production basins of the studied region. These groups were identified by cooperatives' agronomic experts and are characterized by different soil conditions and agricultural practices, i.e. different production scenarios. In a production basin, the agricultural practices and the pedo-climatic conditions can be considered as homogenous. There is no difference in the target market for the studied wheat, we considered only wheat sold on bread flour market. The groups were named after the major soil type of the basin (Table 1).

2.2 System boundaries

The agricultural practices considered in this study are cultivation, sowing, fertilizer and pesticide application and fuel consumption used on fields to produce and harvest the wheat. The wheat seed production phase is considered by using Ecoinvent2.0 life cycle inventory called "Wheat seed IP, at regional storehouse" (Nemecek and Kägi [2007](#page-6-0)). Following the harvest, the transportation of the wheat until the grain silo is considered, as well as the storage of the grain. The consumptions and emissions associated to these different steps are estimated using Ecoinvent data (Nemecek and Kägi [2007](#page-6-0)), adapted to the French agronomic conditions if needed: for agricultural operations (ploughing, sowing, fertilizing and spraying), fuel consumptions were calculated using Arvalis's¹ methodology, described in the methodological guide GES'TIM (Gac et al. [2010\)](#page-6-0). The freshwater ecotoxicity impacts of pesticide applications were assessed for each field separately, using characterization factors (CF) from USEtox (Rosenbaum et al. [2008](#page-6-0)).

2.3 Calculation of freshwater ecotoxicity

We used the USEtox model to calculate aquatic ecotoxicity, as is recommended within the framework of the national experimentation for the environmental display on products that is currently carried out in France. This method is a "consensus model" (Hauschild et al. [2008](#page-6-0)) that allows to characterize the effects of an active ingredient on aquatic ecosystems according to its physical and chemical properties, degradation rates and ecotoxicity results. With the help of this model, characterization factors can be calculated for human toxicity and freshwater ecotoxicity. A characterization factor can be calculated for each chemical. It represents the impact on human toxicity or on freshwater ecotoxicity of the emission of a mass unit of this chemical in the environment. In this study, we consider only the indicator of freshwater ecotoxicity. The CF for freshwater ecotoxicity for a chemical emitted in a compartment is expressed in potentially affected fraction of species (PAF) integrated over time (day) and volume (cubic metre) per kilogramme of chemical emitted.

 $\frac{1}{1}$ Arvalis is a technical institute in charge of applied research on agriculture. GES'TIM is a methodological guide that allows to calculate greenhouse gases emissions in agriculture activity.

This model also provides a database that contains CF already calculated. In USEtox, the ecotoxicological effects of a chemical emitted in the environment (air, soil, water…) suppose a cause–effect chain that allows linking this emission to impacts. Three steps are considered to link an emission with an impact: the environmental fate of the chemical, the exposure and the effects on the ecosystems. To go into USEtox model comprehension in depth, refer to this paper: Rosenbaum et al. [\(2008](#page-6-0)).

We used the USEtox calculator to estimate the CF of the active ingredients that were used in the studied sample but missing in the USEtox database. In this case study, we calculated these CF for 38 active ingredients applied on winter wheat.

The USEtox model does not cover the fate of the active ingredients in the field, right after application (Rosenbaum et al. [2008](#page-6-0)). Consequently, we applied a combination of two different methods to compensate for this: the EMEP–CORINAIR method EMEP/EEA et al. [\(2009\)](#page-6-0) for the emissions in the air and the method of Audsley et al. ([2003](#page-5-0)) for emissions in the soil and in the surface water.

A restricted number of models provide estimates on emissions to all compartments: air, water, soil. Moreover, these models require many specific datasets that were not accessible for this study (Suarez [2005](#page-6-0); Mamy et al. [2010](#page-6-0)) or did not work with French pedo-climatic data (Birkved and Hauschild [2006](#page-6-0)). The EMEP–CORINAIR method allows the calculation of an air pollutant emission factor for an active ingredient, based on its vapour pressure, as described in Table [2.](#page-3-0)

From this method, some emission factors in the air can seem to be very high (95% and 50%), but in fact, most pesticides used by farmers in this study present low vapour pressure, so that the mean fraction of the applied pesticide that is emitted into the air is equal to 23%. Moreover, the USEtox method considers intermediate transfers between the soil, air and water compartments so that the concentration of one chemical in a compartment is evolving with time. For example, the transmission of airborne pesticides into water is considered with mass balance concepts as described in Birkved and Hauschild [\(2006](#page-6-0)) and in Birkved [\(2010](#page-5-0)).

According to Audsley et al. ([2003\)](#page-5-0), the fraction of pesticides applied and emitted into surface water was set at

Table 1 Description of the population

Name of the production	Limy	Stony	Clay	Silty
scenario	soil	soil	loam	clay
Number of fields	2.522	1.020	2.057	1.080
Surface of the sample (ha)	17.651	7.212	12.773	6.858

Vapour pressure (mPa)	Fraction of pesticide applied emitted		
	in air $(\%)$		
p > 10	95		
1 < p < 10	50		
0.1 < p < 1	15		
0.01 < p < 0.1	5		
p<0.01			

Table 2 Fraction emitted in air, depending on vapour pressure of the active ingredient

0.5% of the dose applied. As recommended in Audsley et al. [\(2003](#page-5-0)), no pesticide emission in groundwater was considered. The fraction emitted to soil was calculated as follows:

Fraction of pesticide applied and emitted to soil=100− fraction emitted to air−fraction emitted to surface water.

We fixed a maximum value for the fraction emitted to soil at 85% of the dose applied (Audsley et al. [2003\)](#page-5-0).

3 Results and discussion

3.1 Potential impact on freshwater ecotoxicity of production and storage of 1 kg of winter wheat

Figure 1 shows the potential impact on freshwater ecotoxicity of the production and storage of 1 kg of winter wheat. In this case study, the impact is comprised between 1.9 and 2.3 PAF $m³$ day/kg of wheat, depending on the production scenario. Between 92% and 93% of this impact is due to pesticide use, and the remaining 7% to 8% correspond to the production of seeds and fertilizers and the

Fig. 1 Potential impact on freshwater ecotoxicity of production and storage of 1 kg of winter wheat, according to scenario productions

Fig. 2 Potential impact on freshwater ecotoxicity of pesticide application on winter wheat (box plot: P10, Q1, average, Q3, P90)

storage of the grain. In this way, pesticide use is widely predominant on the whole life cycle of winter wheat. These results are representative of wheat growing in the north east of France, managed with the help of decision-making tools.

3.2 Potential impact of pesticides applied on wheat, per hectare: results and scattering

The freshwater ecotoxicity impacts of pesticide use were assessed for each plot separately. Figure 2 represents the box plot of the results for each production scenario. The results are given in PAF per cubic metre per day per hectare of winter wheat. To avoid uncertainty due to data capture mistakes by farmers in the tool, we considered the 10th percentile as minimum value for the box plot and the 90th percentile as a maximum value for the box plot.

The means of the results for the different production scenarios are quite similar, but the minimum result and the maximum result for the same scenario are very different. The coefficients of variation vary between 257% and 301%, depending on the scenario. So, the scattering of the results for the impact of the only use of pesticides is huge when considering the different fields, but small when considering only the four scenarios (see Fig. 2 and Table 3). All the boxplots in this paper are built in this way: the central dot is the average, the two solid lines represent 25th and 75th percentiles and the extremities represent the 10th and 90th percentiles.

The number of treatments varies between scenarios, with the pedo-climatic situation having an impact on pest and diseases, but the choice of crop protection active ingre-

Table 3 Potential impact on freshwater ecotoxicity of plant protection use for one hectare of winter wheat (Size of the population, mean and standard deviation)

	Silty clay	Clay loam	Limy soil	Stony soil
Number of fields	1.080	2.057	2,522	1,020
Mean freshwater ecotoxicity	16.125	17.574	19.460	15.704
Standard deviation	44.894	50,407	50,070	47,322

Fig. 3 Active ingredients substitution effect on freshwater ecotoxicity of pesticides used on winter wheat (P10, Q1, average, Q3, P90)

dients has a much bigger impact on the ecotoxicity score than the number of treatments. This explains the high variability between plots. This importance of the active ingredient choice is due to the fact that USEtox CF highly vary according to the active ingredients. The active ingredients with the highest impact were identified and replaced by other active ingredients having the same agronomic role but different potential impacts on freshwater ecotoxicity.

3.3 Active ingredients replacements and effects on the results

One herbicidal active ingredient, one fungicide active ingredient and one insecticidal active ingredient were identified as preponderant in the freshwater ecotoxicity score of pesticide use on winter wheat. These active ingredients have a high CF compared to others that can have the same agronomic role. With the help of plant protection and agronomic experts, we identified substitute active ingredients for these three active ingredients with a high CF. The substitution conditions were: to identify substitute active ingredients with the same role, the same efficiency on the targets and the same order of price for the farmers. These three active ingredients were replaced in the

databases, and calculation of freshwater ecotoxicity was done on pesticide use on winter wheat, with the substituted active ingredients.

For example, the insecticidal active ingredient that is replaced has a CF of 4,480 PAF $m³$ day/g of active ingredient applied in the field. This active ingredient is replaced by another plant protection product that contains two different active ingredients, with the same agronomic role and the same efficiency, that have CFs of 1,200 and 0.31 PAF m^3 day/g of active ingredient applied. The fungicide active ingredient that is replaced has a CF of 62 PAF $m³$ day/g of active ingredient applied in the field. This active ingredient is replaced by another plant protection product that contains two different active ingredients, with the same agronomic role and the same efficiency, that have CFs of 1.05E−2 and 2.80E−2 PAF m³ day/g of active ingredient applied. The herbicide active ingredient that is replaced has a CF of 9.01 PAF $m³$ day/g of active ingredient applied in the field. This active ingredient is replaced by another plant protection product that contains three different active ingredients, with the same agronomic role and the same efficiency, that have respectively CFs of 1.44E−5, 4.61E−4 and 5.66E−7 PAF m³ day/g of active ingredient applied.

In the studied region, we observe more than 100 different active ingredients for plant protection used by farmers. The substitution of only three active ingredients (one herbicidal active ingredient, one fungicide active ingredient and one insecticidal active ingredient) contributes to a decrease of about 50% of the average freshwater ecotoxicity, regardless of the scenario (Fig. 3). The 10th percentile remains almost unchanged after the substitution, while the 90th percentile is strongly reduced. The fields with a high impact on freshwater ecotoxicity are indeed those on which active ingredients with high CF were used. So, the substitution has a predominant role in the reduction of the impact of the field with the highest ecotoxicity score.

3.4 Explanation of high variability between plots

The results of freshwater ecotoxicity impacts of pesticide use in this study present a high variability because of the

very high variability between the CF of active ingredients. For example, in this study, before active ingredient replacement, the lowest CF for an active ingredient emitted in water is equal to 1.6E−46 PAF m³ day/kg of active ingredient emitted in freshwater, while the highest CF for an active ingredient emitted in water is equal to 4.9E+8 PAF $m³$ day/kg of active ingredient emitted in freshwater. The mean CF of active ingredients used in this study, for freshwater emissions, is equal to 9.3E+6 PAF $m³$ day/kg of active ingredient emitted, and the standard deviation for the same population is equal to 5.7E−7. Accordingly, the model USEtox can give very different CF for two different active ingredients, which can explain the significant decrease in freshwater ecotoxicity impact for substitution active ingredients. This underlines the importance of the active ingredient choice by farmers on the impact of wheat production on the freshwater ecotoxicity indicator.

3.5 Comparison of emission factors in air with experimental measurements

The methodology used in this study to calculate emission factors in the air EMEP/EEA et al. ([2009](#page-6-0)) can be compared with experimental volatilisation measurements in France in a study carried out by Bedos et al. (2009). In the paper of Bedo et al. (2009), three herbicidal active ingredients' volatilisations in field are measured. These active ingredients are atrazine, alachlor and trifluralin. Emission factors were calculated for these three substances using the same EMEP–CORINAIR method EMEP/EEA et al. [\(2009](#page-6-0)) as in this study on wheat. Results are presented in Table [4](#page-4-0).

Differences between measured quantities emitted in the air and calculated quantities emitted in the air for these three active ingredients are quite high for one substance especially: measured and calculated losses in the air are 4.4 versus 27.5 g ha⁻¹ for atrazine, 34.4 versus 220 g ha⁻¹ for alachlor and 357 versus 440 g ha^{-1} for trifluralin. Nevertheless, the ranking between the three substances is the same for measured and calculated emitted quantities. Bedos et al. (2009) suggested that at the end of the measurements, the quantity of active ingredients that still remained in the soil suggested that further volatilisation could occur, which could explain the high numbers of our calculated emitted quantity compared to measurements.

However, the EMEP-CORINAIR method EMEP/EEA et al. [\(2009](#page-6-0)) is well adapted to LCA practitioners because of its simplicity, even if it could be quite imprecise because of different classes of vapour pressure. For example, alachlor and trifluralin are in the same class of vapour pressure: [1 mPa; 10 mPa] but each at a class extremity, leading to differences between measured emissions that are not noticed with calculated emissions.

4 Conclusions and perspectives

The combination of InVivo's databases that constitute an important and complete dataset of real agricultural practices and the USEtox model that offers characterization factors calculated for each molecule used offers a precise and broad point of view on potential impacts of agricultural practices on freshwater ecotoxicity. This enables us to underline its sensibility to pesticides practices data and then the particular importance that should be given to data collection.

Using fixed emission rates for freshwater emissions, whichever pesticide is used, constitutes the main limit of this study. Models like PESTLCI (Birkved and Hauschild [2006](#page-6-0)) can calculate emission factors for different compartments depending on pedo-climatic situation, date of application and application technique, but are not easily transposable to the French climatic and pedologic situation. Moreover, the other models such as PRZM (Suarez [2005;](#page-6-0) Mamy et al. [2010\)](#page-6-0) require data with a level of detail that is not reasonably accessible for LCA practitioners, apart from the research context. This is why, waiting for a better solution, we used the combined Audsley's and EMEP-CORINAIR methods (Audsley et al. 2003; EMEP/EEA et al. [2009\)](#page-6-0). The next step to improve these results will be using a model such as PESTLCI adapted or adaptable to French conditions, in order to have differentiated emission factors for the molecules. This paper is a way to get the message across the LCA research community that agricultural LCA practitioners need results and models to tackle the problem of pesticide emissions quantification on the field.

Acknowledgements The authors wish to acknowledge the plant protection experts who helped to lead the active ingredients' substitution: Axel Olivier, fungicide protection expert; Céline Denieul, herbicidal protection expert, and Luc Messean, insecticidal protection expert. We also wish to acknowledge Caroline Dizien and David Durand Delacre for the rereading of the paper.

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