

Modeling pesticides emissions for Grapevine Life Cycle Assessment: adaptation of Pest-LCI model to viticulture

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ABSTRACT

This paper presents a tailored version of PestLCI 2.0, the most advanced life cycle inventory model for quantification of organic pesticide emissions from arable land, customized to appropriately account for viticulture specificities affecting pesticides emissions from vineyards. PestLCI 2.0 customization is further supported by the calculation of USEtox™ freshwater ecotoxicity characterization factors for active ingredients relevant in viticulture. Case studies on two different vineyard management systems illustrate PestLCI 2.0 model application. The customization of the PestLCI 2.0 model includes addition of 29 active substances, 9 application techniques, interception by a dual canopy (vine /grass cover), new soil and climate databases and further account of multiple vinerow treatment. Four substances dominate the overall toxicity profiles. Comparing the results obtained with PestLCI 2.0 with existing static emission quantification approaches results reveals that PestLCI 2.0 yields considerable lower emission loads and consequently, lower toxicity impact burdens. The issue of accounting for inorganic substances is discussed.

Keywords: plant protection product, LCA, vineyard, modelling, emissions, fate

1. Introduction

Wine production and hence viticulture are an important economic and cultural sector in main parts of the world including Europe. Viticulture is also a major pesticide consuming sector with app. 20 kg formulated pesticides/ha/year (of which app. 15 kg/ha are elemental sulfur) within the European Union (Endure 2010).

Pesticides emissions are therefore a crucial topic to be addressed when performing wine and/or grape production related life cycle assessments (LCAs). Due to the lack of specific inventory models suited for pesticide emission quantification, most of the published wine LCA studies either neglect pesticide emissions (Point et al. 2012; Pattara et al. 2012; Bosco et al. 2011; Ardente et al. 2006), simply assume that 100% is emitted to the soil (in accordance with the default Ecoinvent approach applied for pesticides (Nemecek and Schnetzer 2011)) or propose a fixed partition as (Neto et al. 2012) with 75 % of pesticides emitted to soil and 25% to the air.

PestLCI (Dijkman et al. 2012; Birkved and Hauschild 2006) is currently the most advanced LCI model for pesticides emissions quantification from arable land (van Zelm et al. 2014). Despite the fact that the model has been applied in wine/grape production LCAs (Villanueva-Rey et al. 2014; Vázquez-Rowe et al. 2012), PestLCI 2.0 still does not take into account certain viticulture specificities such as double cropping systems, vertical application techniques etc. which differentiate viticulture from other crops and influence the emission patterns of pesticides. Characterization of the impacts from pesticide related emissions specific to viticulture and fruits or vegetable crop production furthermore requires characterization factors for these chemical compounds.

This paper presents a PestLCI 2.0 version customized to appropriately account for viticulture specificities affecting the emission quantities and patterns of pesticides from vineyards. The application of the customized inventory model is illustrated by calculation of potential ecotoxicity impacts through combination of emission quantities and freshwater ecotoxicity characterization factors calculated using the USEtox™ characterization model. The combination of the PestLCI 2.0 and USEtox™ models is illustrated through two case studies on vineyard technical management routes¹ (Renaud-Gentié et al. 2014; Renaud-Gentié et al. 2013).

¹ technical management routes (TMRs): logical successions of technical options designed by the farmers (Renaud-Gentié et al. 2014))

2. Methods

2.1. Pest LCI

PestLCI is a dedicated inventory model intended to provide emission quantities for use in relation to the characterization of chemically induced impacts caused by emissions of pesticides from arable land/technosphere to the environment/ecosphere. The most recent version of the model, version 2.0, is described in Dijkman et al. (2012). This version of the model covers app. 90 active ingredients of various types of pesticides, 25 European climate profiles and 7 European soil profiles.

Despite the rather extensive coverage in terms of pesticides, climates and soils, the most recent model version was developed with conventional agriculture in mind and viticulture was hence not addressed specifically. In order to improve the viticulture specificity of the model, PestLCI version 2.0 was updated with 28 pesticides frequently used in European viticulture, 5 French soil profiles, 22 French temperate maritime climate profiles, 34 crop stages and cover crop combinations + 13 direct spraying situations as well as 9 pesticide application techniques typically applied in European viticulture.

2.2. Identification of specific needs for pesticides emissions modeling in viticulture

2.2.1. Pest and weed management in viticulture

The main pests damaging the vine canopy are primarily the fungi downy mildew (*Plasmopara Viticola*) and powdery mildew (*Uncinula Necator*), which necessitate fungicide treatments. The other fungi and the main insect pests (moths, leafhoppers and phytophagous mites) are not systematically treated. Vineyard management includes also weed control, since weed presence can affect vine growth by competition for water and nutrients. Most of these pests require specific pesticide active ingredient substances (ai.s). The risk of resistance acquisition by the pests implies frequent change of ai.s, in conventional² viticulture especially for ai.s presenting a single-site action. Vineyard treatment programs therefore usually involve a variety of pesticide ai.s. This is however not the case in organic viticulture, where the fungicides used (primarily copper and/or sulfur based fungicides) have multi-site action, while weeds in organic viticulture are mechanically controlled.

2.2.2. Active substances

Vineyard management involves, in French context, on average 14 to 16 pesticide applications per year at full recommended application rates (Mézière et al. 2009; Ambiaud 2012b) with a high interregional and inter-annual variability mainly related to climatic conditions and winegrowers practices. Organic and inorganic or partially inorganic pesticides ai.s are used by viticulture.

Conventional pest management in viticulture relies on generic farming organic pesticides ai.s, but also on more crop specific organic pesticide ai.s typically used on vegetables or in orchards. All these crop specific active substances were not included in PestLCI 2.0 version presented by (Dijkman et al. 2012). The substances used in the cases studied in the project at hand were listed. Compilation of data on the properties of these substances used in viticulture, however missing in the PestLCI 2.0, was conducted applying specialized chemical databases: “e-phy” (MAAF and ONPV 2013) for correspondence between commercial name and active substance, “PPDB” (University-of-Hertfordshire 2013), “Toxnet” (US-National-Library-of-Medicine 2013) as well as “Chemspider” (Royal-Society-of-Chemistry 2013) for main chemical and physical characteristics. Data gaps were compensated for applying the Quantitative Structure-Activity Relationships included in the EPI SuiteTM (US-Environmental-protection-Agency 2012).

However, conventional and organic viticultures also apply inorganic sulfur (S8) and copper-based fungicide ai.s. to manage powdery mildew (mainly sulfur) and downy mildew (mainly copper). They also use other inorganic ai.s like Ammonium thiocyanate (herbicide) or partially inorganic like Fosetyl-Al (fungicide). However, PestLCI 2.0 is designed only for modelling of organic pesticide a.i. emissions. For this reason, inorganic pesticides were not included in this study.

² « Conventional » is used in this paper to designate non-organic plant protection practices

Some pesticide a.i.s applied in the studied vineyards, especially organic vineyards are derived from micro-organisms like Spinosyn, or plants like Pyrethrum. The physical-chemical and fate properties of these pesticide a.i.s were found in Bio-Pesticide DataBase (BPDB) (University-of-Hertfordshire 2012) and some of the previously cited databases. A second fraction of “others pesticides and pesticide ingredients” are substances like algae extracts and pesticide formulation additives which are not considered in this study, due to lack of information about the nature and quantity of these substances. Formulation additives may however despite of their exclusion of this study, contribute considerable to toxicity of the pesticide formulation (Brausch and Smith 2007).

2.2.3. Spraying equipment

Vertical shoot positioning is the most frequent training system³ for vineyards in France and is found in many other wine producing countries. The case studies assessed in the paper at hand only cover vertical shoot positioning trained vineyards.

The types of spraying equipment involved in viticulture are multiple, which makes the task of modeling their individual characteristics a challenge. Herbicides are most often applied using specific sheltered booms to avoid herbicide drift and hence deposition on vine leaves (which would damage/kill the wines). We chose to model these application techniques as “soil incorporation” in Pest LCI since they induce very low drift. The sprayers designed for canopy and grapes spraying can use different modes of droplets production:

- *non air-assisted spray*, the droplets are formed by the acceleration of the liquid under pressure in the nozzle, and applied to the leaves by the pressure,
- *airblast*, the droplets are formed through nozzles, and are then subsequently transported to the leaves by an air flux which further shakes the wine leaves, thereby facilitating the penetration of the substance into the canopy,
- *pneumatic* where air accelerated to app. 300km/h meets the liquid containing the pesticide formulation and fragments the solution into very fine droplets and conveys it to the leaves.

Different shapes of the ventilators and of the sprayers themselves lead to different patterns in terms of spraying quality and drift generation. These different shapes also permit either a direct spraying of each face of the canopy or a spraying from the top of the rows.

A last type of sprayer was designed for drift reduction: the tunnel sprayer where specific panels prevent from drift and collect the non-intercepted spray mixture and recycle it for re-use.

PestLCI 2.0 takes into account the type of sprayer in order to quantify the drift calculations through drift curves. Sprayers representing the above presented application techniques were however not available in PestLCI 2.0. In the present customization, 9 sprayers with different modes of action were included. For the customization and the viticulture specific application techniques we used data from (Codis et al. 2011) who conducted drift tests according to International Organization for Standardization (ISO) protocol (ISO 2005), on different vineyard spraying equipment types in France. The sprayers successfully tested by (Codis et al. 2011) plus a tunnel sprayer tested by (Ganzelmeier 2000) were included in the viticulture customized PestLCI 2.0 version. Defining within this list of the 9 sprayers, the ones that are the more similar to the ones we have in our case studies was done through discussion with the author S. Codis (Codis 2014).

Since the aforementioned drift tests used to derive spray drift curves were conducted on vines with one leaf area, PestLCI 2.0 was adapted in order to correct for spraying on vines with different leaf areas. Modelling of custom spray techniques covering various adaptations of existing spraying equipment is considered beyond the scope of this paper.

According to the type of sprayer, the winegrower can choose to spray 1 to 4 rows of vines simultaneously. The number of rows treated plays a role in wind drift calculation in PestLCI 2.0. It has been taken into account using the parameter “nozzle distance on the model”, the distance entered being the actual width (in meter) treated at the same time.

³ Training system : type of trellis and shoot positioning resulting to a given shape of the vine canopy and position of grapes.

2.2.4. Accounting for primary distribution in double cropping system

The primary distribution process is defined in PestLCI by 3 factors: wind drift (f_d), pesticide deposition on soil (f_s) and pesticide deposition on leaves (f_l) (Birkved and Hauschild 2006). The two latter are based on (Linders et al. 2000) interception factors for single crops at different growing stages.

Concerning interception by vine canopy, PestLCI 2.0 includes interception values for vine at four different development stages I, II, III, and IV based on (Linders et al. 2000). A stage 0 has been added to take into account situations of leafless vines. The interception factor has been estimated from the orchard dormancy stage interception factor (0.2) given by (Linders et al. 2000) with a division by 2 due to the difference of perennial parts importance between fruit trees and vines. The value of f_l for vine 0 was therefore set to 0.1.

On-field measurements of spraying mixture deposition and losses on vineyards were made by Sinfort (Sinfort 2014) (Sinfort et al. 2009) and on artificial vineyard by (Codis 2014). Distribution ratios of spray mixture between vine canopy, soil and air at 2.5 m above the soil were obtained by these authors in vineyard conditions similar to the ones we study (rows width, types of sprayers). The fractions going to air during spraying measured by (Codis 2014) and (Sinfort et al. 2009) were considered for introduction in PestLCI 2.0 as being i) partly conveyed by wind drift out of the parcel (i.e. advective transport), and ii) partly falling back on vegetation and bare soil of the parcel (i.e. sedimentation). This is because no quantification of direct volatilization is possible (Jensen and Olesen 2014) due to the complexity of drivers combination (properties of the spray liquid, drops size and drops surrounding conditions)(Gil et al. 2007) and the lack of available data for some of them. As PestLCI 2.0 calculates the quantity of drifted pesticide on the basis of the dose applied and before calculating leaf interception, we decided to apply a drift quantity correction ratio based on the pesticide fraction going to air. Full vegetation (stage III) was given the 1:1 ratio because sprayers drift curves were established on that stage.

For accounting of direct spraying with hand hose in early stages or young vineyards, and direct spraying on grapes, 13 specific interception factors were defined through expertise.

Cover cropping on vineyard soil is a developing management scheme with nearly half of French vineyard temporarily or permanently covered (Ambiaud 2012a). It offers multiple advantages, provided the competition for water and nitrogen isn't excessive for the vineyard (Celette et al. 2009). This second canopy under the vineyard (e.g. spontaneous species, oats, clover or fescue) contributes to pesticide interception (primary distribution) and fate (secondary distribution). The interception by the cover crop varies according to the width of the cover crop strips estimated in percentage of the width of the vine inter-row, and according to cover crop canopy density.

In the case of mixed cropping (vine + cover crop), a complementary interception factor (f) needs to be added for cover crop. The structure of PestLCI 2.0 being fixed with 3 f entries, a combined f has been calculated from f_{vine} and $f_{covercrop}$. Based on calculation routines, 34 combined interception factors are now available in the customized PestLCI 2.0 model covering the most current situations spanning possible combinations of vine development stages, cover-crop strip width and cover crop canopy density. Examples of such combinations are given in Table 1.

Table 1: Examples of combined interception factors for vine/cover crop mixed cover (f = interception factor)

Stage	cover density	% of soil surface covered by grass	f_{vine}	$f_{covercrop}$	% spray lost in air	% intercepted by vegetal soil cover (calculation)	f_{global}
0	none	0	0.1	0.3	30%	0%	0.10
II	weak (30%)	100%	0.5	0.3	30%	6%	0.56
II	high (70%)	80%	0.5	0.7	30%	11%	0.61
III	average (50%)	100%	0.65	0.5	25%	5%	0.70

2.2.5. Databases

Site specific climatic profiles appropriately addressing the case study areas were introduced in PestLCI 2.0: two sets of 30 years average 1971-2000 and 1981-2010 for the Beaucouzé Station, and for the five stations of the Middle Loire Valley, being the closest to the observed parcels, data for 3 years of production i.e. October n - September n+1, for 2009-2010 to 2011-2012, a set of averaged months over the 3 years is also available. Climat-

ic data were provided by Météo France. The soils of the modelled parcels were characterized through measured data and observations, in accordance with the PestLCI 2.0 data requirements, and entered in PestLCI 2.0.

2.3. Case study

2.3.1. Choice and main characteristics

Two quite different technical management routes (TMRs) of *Chenin Blanc* cultivar in the middle Loire Valley (France), were observed during the production year 2010-2011. The prevailing Loire Valley climate is temperate maritime according to the classification used in PestLCI 2.0. This study is focused on vineyard TMRs designed for Protected Denomination of Origin (PDO) dry wine production from this cultivar. The case studies were chosen within the 5 types of vineyard TMRs resulting from a detailed survey and analysis of existing vineyard management practices in the area (Renaud-Gentié et al. 2014): 1 “systematic synthetic chemical use and limited handwork”, 2 “moderate chemical use”, 3 “minimum synthetic treatments and interventions”, 4 “moderate organic”, and 5 “intensive organic”(organic with many interventions and treatments).

The two cases presented here: TMRs 1 and 3 are real situations representing respectively type 1 and 3. Organic TMRs are not studied here because their treatment programs include mainly or exclusively inorganic pesticide a.i.s. No surface water body lies at less than 100m of the parcels. The 2 plots are not drained nor irrigated.

In comparison to the 30 year average (1981-2010) of the area, the climate of the focus year is: i) a little warmer (0.2°C above the annual average) with a warmer spring but a cooler summer, ii) much drier especially during the growth season of the vine.

TMR 1’s plot climate is described by Blaison-Gohier weather station, is on the soil “UTB131” according to the regional cartography of vineyard soils, with 5% slope. TMR 3’s plot climate is described by Fontaine-Guérin station. Its slope is 3%, and soil is “UTB35”. Field width and length were put at 100m for the two plots. Vineyard pest management programs, spraying equipment and pesticide a.i.s used by the growers, as well as canopy development stage and grass cover density and extent are described in table 2.

Table 2: Characteristics of pesticide a.i.s applications for 2011 on TMRs 1 and 3. *In grey: the inorganic and partially inorganic pesticide a.i.s that were not included in this study. *: new entries in PestLCI 2.0. ■ needed a new CF in USETox™*

	pesticide a.i.s	Application rate	Crop type + development stage	Month of application	Application method	width treated at a time
TMR1	*Amitrole	0.79	Grass I - all phases	april	sheltered boom	1.85
	Aclonifen	0.31	Grass I - all phases	april	sheltered boom	1.85
	Sulfur	5.89	*Vines II - h80% grass	may	tunnel sprayer	1.85
	Folpet	0.74	*Vines II - h80% grass	may	tunnel sprayer	1.85
	Fosetyl-Aluminium	1.47	*Vines II - h80% grass	may	tunnel sprayer	1.85
	*Fluopicolide	0.12	*Vines II - h80% grass	may	airblast sprayer	7.4
	Fosetyl-Aluminium	1.75	*Vines II - h80% grass	may	airblast sprayer	7.4
	*Proquinazid Technique	0.05	*Vines II - h80% grass	may	airblast sprayer	7.4
	*Tétraconazole	0.03	*Vines III - a80% grass	june	airblast sprayer	7.4
	*Indoxacarbe	0.04	*Vines III - a80% grass	june	airblast sprayer	7.4
	copper oxychloride	0.73	*Vines III - a80% grass	july	airblast sprayer	7.4
	copper sulfate	0.18	*Vines III - a80% grass	july	airblast sprayer	7.4
	*Cymoxanil	0.12	*Vines III - a80% grass	july	airblast sprayer	7.4
	Mancozèbe	0.40	*Vines III - a80% grass	july	airblast sprayer	7.4
TMR3	Glyphosate	0.54	Grass I - all phases	march	sheltered boom	1.95
	*Amitrole	0.92	Grass I - all phases	march	sheltered boom	1.95
	ammonium thiocyanate	0.86	Grass I - all phases	march	sheltered boom	1.95
	*Flazasulfuron	0.02	Grass I - all phases	march	sheltered boom	1.95
	Glyphosate	0.09	Grass I - all phases	may	sheltered boom	1.95
	■Trifloxystrobin	0.06	*Vines II - a50% grass	may	pneumatic sprayer side by side	7.8
	■Trifloxystrobin	0.06	*Vines III - a50% grass	june	pneumatic sprayer side by side	7.8
	Diméthomorph	0.18	*Vines III - a50% grass	june	pneumatic sprayer side by side	7.8
	Mancozèbe	1.20	*Vines III - a50% grass	june	pneumatic sprayer side by side	7.8
	*Difénoconazole	0.03	*Vines III - a50% grass	july	pneumatic sprayer side by side	7.8
	*Meptyldinocap	0.21	*Vines III - a50% grass	july	pneumatic sprayer side by side	7.8

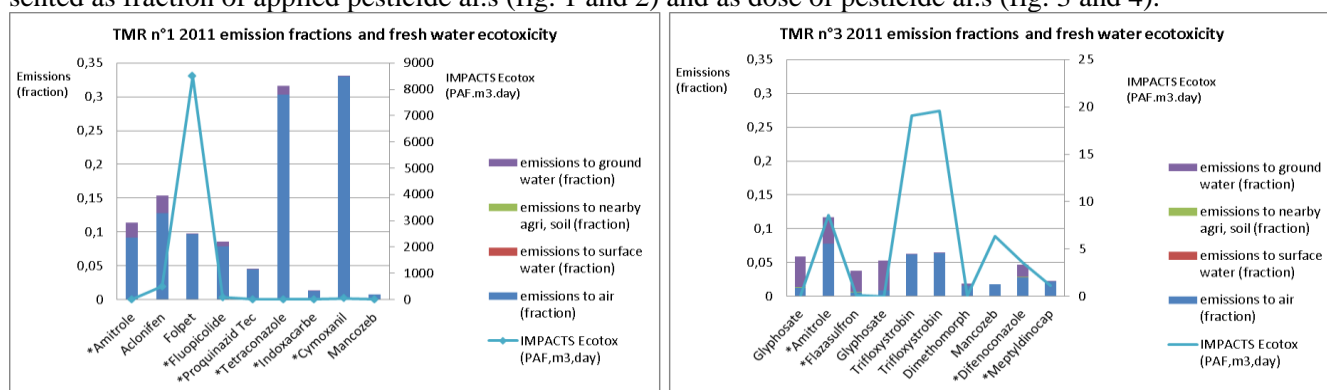
2.3.2. Calculating characterization factors in USEtox™

Characterization factors (CF) are needed to quantify the potential environmental impact from emissions of the life cycles of products and systems in LCA. CFs are substance and compartment specific and CFs for each of the emitted ai.s of the case study for compartments air, surface water and agricultural soil⁴ are thus needed. We choose USEtox™ as characterization model since it was developed as a scientific consensus model, to represent the best application practice for characterization of toxic impacts of chemicals in LCA (Hauschild et al. 2008) and since its database (v. 1.01) covers ~2500 chemicals with calculated characterization factors for freshwater ecotoxicity (Rosenbaum et al. 2008). Some of the ai.s were not covered by the database and we therefore applied the USEtox™ model to calculate them. USEtox™ requires a number of chemical and physical properties in addition to toxicity data. Primary and secondary sources for these data are available upon demand to the authors.

3. Results

3.1. Emissions and Freshwater ecotoxicity on the case study

Pesticide ai.s emissions were calculated by PestLCI 2.0 for each organic substance application. They are presented as fraction of applied pesticide ai.s (fig. 1 and 2) and as dose of pesticide ai.s (fig. 3 and 4).



Figures 1 and 2: fraction of applied pesticide ai.s emitted in the 4 compartments: fresh and ground water, nearby agricultural soil and air (left axis) and the resulting freshwater ecotoxicity (right axis, scales adapted to results)

The total emission fractions do not exceed 0.35, and are lower than 0.15 for most of the pesticides. The emissions loads are dominated by air emissions in figure 1, followed by ground water emissions. In figure 2, groundwater emissions dominate, for the 4 herbicides. Emissions to nearby agricultural soils are negligible, and thus don't appear on the charts. The absence or quasi-absence of freshwater emissions are due to the absence of water body around the parcels.

The higher total emission fractions relate primarily to Tetraconazole (fungicide of the Triazole group), Cy-moxanil (fungicide of Cyanoacetamide Oxime group) and Mefenoxam (fungicide of the Phenylamide group). These fungicides are emission load wise followed by two herbicides: Aclonifen (Diphenyl ether group) and Amitrole (Triazole group) and another fungicide: Folpet (Phtalimides group).

In some cases, the same substance is applied under two different conditions. Amitrole, for example, is applied with the same type of boom (herbicide sheltered boom) and on the same canopy (grass). However, the emissions of this compound vary according to the conditions of application (month of application and soil vary). An application of Amitrole in April (figure 1) compared to an application of Amitrole in March (figure 2) shows lower emissions to air for the early application, while emissions to groundwater are higher for the latest application.

⁴ USEtox contains no ground water compartment. Ecotoxicological impacts in freshwater from chemical emissions to groundwater are considered negligible and thus not further considered in this study.

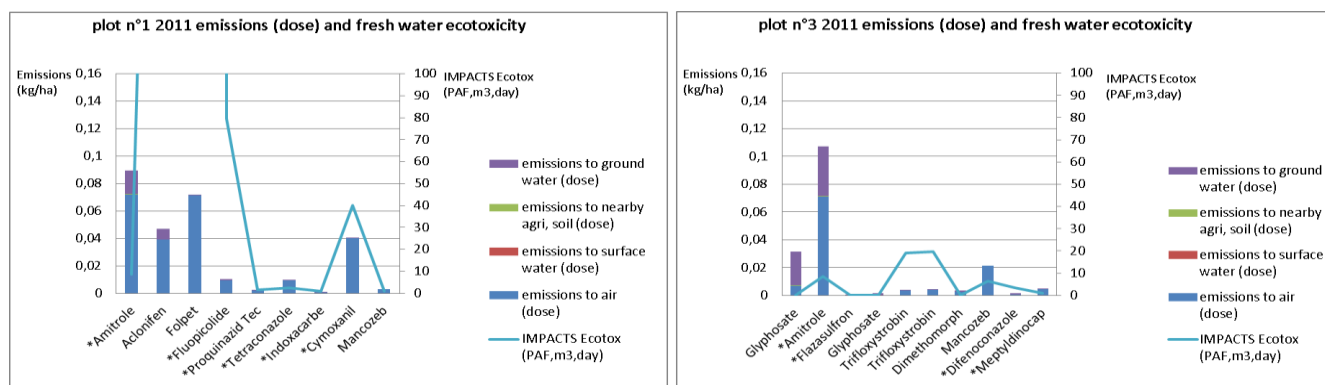


Figure 3 and 4: Quantity of applied pesticide ai.s emitted in the 4 compartments and freshwater ecotoxicity (Impacts Ecotox (same values as fig 1 and 2) scale was fixed here to a maximum of 100 to see smaller differences)

When expressing the emissions in kg/ha, see figures 3 and 4, the quantity emitted to the ecosphere per application is not higher than 0.12 kg/ha. Amitrole dominates the emissions air in both scenarios (fig. 3 and 4), followed by Folpet and Aclonifen.

Freshwater ecotoxicity (FwEtox) was calculated applying USEtox™ characterization factors. Figures 1 and 2 reveal considerable differences for the different application times. In figure 1, FwEtox is dominated by Folpet (8000 PAF·m³·day), Aclonifen (500 PAF·m³·day), Fluopicolide (80 PAF·m³·day) and Cymoxanil (40 PAF·m³·day). The high impact from Folpet emissions is primarily caused by emissions to air and can be explained from a combination of the substance’s relatively low vapor pressure (meaning that a substantial amount of emissions of Folpet to air ends up in the freshwater compartment) and its relatively high toxicity to freshwater organisms. TMR3 shows a much lower total FwEtox (58.5 PAF·m³·day) than TMR1 (9132 PAF·m³·day).

3.2. Comparison with static emission quantification approaches

The Ecoinvent approach applied for pesticides is to consider that 100% is emitted to the soil (Nemecek and Schnetzer 2011), (Neto et al. 2012) in their LCA of Portuguese wine Vinho Verde propose a static partition as with 75 % of pesticides emitted to soil and 25% to the air. Table 2 compares results between the 3 approaches.

Table 3: Comparison of pesticides emissions calculated by PestLCI 2.0, Ecoinvent and Neto et al. (2012) approaches and FwEtox calculated with USEtox™ characterization factors

Emissions	average fraction emitted	standard deviation on fractions
PestLCI 2.0-emissions to air	7.39E-02	9.30E-02
PestLCI 2.0-emissions to surface water	0	0
PestLCI 2.0-emissions to nearby agri. soil	8.06E-05	1.19E-04
PestLCI 2.0-emissions to ground water	1.32E-02	1.68E-02
PestLCI 2.0-total emissions	8.72E-02	9.21E-02
100% emitted to soil (Ecoinvent)	1	0
75% emitted to soil (Neto et al 2012)	0.75E-01	0
25% emitted to air (Neto et al 2012)	0.25E-01	0
Impacts	average impact	standard deviation on impacts
Impacts FwEtox PestLCI 2.0 (PAF·m³·day)	4.84E+02	1.94E+03
impacts FwEtox Ecoinvent (PAF·m³·day)	1.52E+04	6.46E+04
impacts FwEtox Neto et al. (PAF·m³·day)	1.26E+04	5.35E+04

In the present cases, the average of total emission fraction modelled with PestLCI 2.0 is more than 31 times lower than the total soil emission fraction estimated by Ecoinvent approach. The average PestLCI 2.0 modelled emission fraction to air is 3.4 times lower than the total emission fraction to air estimated by Neto et al. (2012) approach. This leads to differences in FwEtox estimates: 31 times lower with PestLCI model than Ecoinvent ap-

proach, and 26 times lower with PestLCI model than with Neto et al. (2012) approach. Very high standard deviations must be noticed on FwEtox, due to high differences in the ai.s' FwEtox potential.

4. Discussion

While having been intended mainly for arable crops, PestLCI 2.0 inventory model, due to its rather flexible framework, has here been adapted for viticulture without compromising the model framework. The calculation of toxicological impact potentials, beyond emission load quantification, was further complicated by ai.s not covered by the USEToxTM database, thus necessitating the calculation of CFs using the USEToxTM mode.

The case study results show that emission fractions vary in a large extent due to the ai.s properties and parcel and application conditions. High emissions fractions for most of the ai.s are compensated by very low application doses (cymoxanil, teaconazole) leading to moderate emissions (dose) but the ecotoxicological profile of the ai.s then has high importance on the final FwEtox results as shown by the FwEtox of Folpet and Aclonifen. Multiple factors differentiate the two case vineyards TMR1 and 3. The main factors are considered to be soil, sprayer equipment and type of pesticides applied. TMR1 shows higher emissions fractions than TMR3, however the total emission load is lower because of the low doses applied for some substances. Characterization through USEToxTM reveals different results for the two cases, mainly due to the high ecotoxicity potential of Folpet and to a lesser extent, of Aclonifen, even if both ai.s are applied via sheltered boom and tunnel sprayer (both limiting wind drift) (TMR1).

Inorganic pesticide ai.s, which are not modelled here, were also applied to the case vineyards: five applications for TMR1 including copper based ai.s and one application for TMR3 (Table2). The copper based pesticide ai.s are expected to further increase the FwEtox of TMR1 if included (Mackie et al. 2012; Vázquez-Rowe et al. 2012). A comparison of the present TMRs FwEtox profiles with the results obtained by (Vázquez-Rowe et al. 2012) with PestLCI 1 in Galician vineyards shows very good performance of the present TMR. Hence, TMR1's FwEtox is half of the lowest FwEtox mentioned by this author (Copper impacts removed) while TMR3's FwEtox is 400 times lower as this author's lower result.

Huge differences were found between the two static approaches (Ecoinvent and Neto et al. 2012) and PestLCI 2.0 based emission quantification. Accounting for the sole emissions that cross the parcel borders is a first element lowering the quantity of emitted pesticides as modelled by PestLCI 2.0, compared to the other approaches tested. However that is not the only cause of lower emissions and FwEtox; considering, for these emissions calculations, processes of evaporation, runoff and leaching, canopy influence, including the actual properties of the pesticide ai.s applied, of soils and sprayers allows for a more accurate adjustment of estimates to the real phenomenons. Degradation of pesticide ai.s and their uptake by the plants are actual processes that aren't considered in the static approaches tested, but accounted for in PestLCI 2.0 (Dijkman et al. 2012). The uptake of pesticides in crops including edible parts, is in PestLCI only considered as a fate/removal process and hence export from the field of pesticides via crops and crop residues is not considered nor quantified. Plant pesticide uptake processes are complex systems of coupled processes demanding dedicated models such as DynamiCROP (see e.g. (Fantke et al. 2011)).

In organic viticulture, sulfur and copper are the only means available to manage respectively powdery and downy mildew, and represent important quantities of applied pesticides. Sulfur and copper are not available in PestLCI 2.0 as the model is designed for modelling of organic pesticide ai. emissions. Thus, a comparison between conventional and organic viticulture or inclusion of organic managed cases in a study cannot be dealt with solely through PestLCI 2.0; a model similar to PestLCI is needed for inorganic pesticides. Considering the complex chemistry of inorganic chemicals, such a model will however have to deal with multiple species nature of inorganic chemicals in order to appropriately reflect the behaviour of these chemicals in soils.

PestLCI 2.0 could be improved by further developments of the accounting of airborne drift, which can be considerable (Jensen and Olesen 2014) but the complexity of the phenomena (Gil et al. 2008) and the lack of (generic) data are considered major obstacles for this improvement. More or less for the same reasons, pesticide metabolites are not accounted for in the present version of PestLCI 2.0. Accounting for application parameters as sprayers' speed, droplets size, temperature, relative humidity would be ideal for further refinement of the modelling of the spray mixture behaviour and fate, but these parameters are too difficult to obtain from the growers, and would further entail an even more complicated inventory.

High percentages of stones can be found in many vineyard soils; and modify water flow in the soil. These aspects could not be included in the present customization of PestLCI 2.0. However we recommend improvement of the way soil texture affects macropore transport in PestLCI 2.0 as an important issue to be considered in the coming PestLCI versions.

PestLCI 2.0, calculations must be carried out for each pesticide a.i.s and application and thus remain a tedious task. Ideally, a possible connection with an external Excel database could potentially facilitate the automation (batch) of calculation and further pave the road for more detailed sensitivity analyses.

5. Conclusion

The PestLCI 2.0 customized version for viticulture, presented in the paper at hand, facilitates the calculations of emission loads for vertically trained vineyards with a wide range of sprayers and further provides a considerable PestLCI pesticide database update (even if non-exhaustive), of viticulture specific pesticides a.i.s, and is complemented by the corresponding UseTOX™ FwEtox characterization factors. A range of rather important specificities of viticulture that were not included in PestLCI 2.0. has been added like: i) specific sprayers drift characteristics, ii) the presence of a secondary canopy (cover-crop), iii) specific data like specific pesticide a.i.s in the PestLCI database.

Application on two different case studies shows that emissions differ from a pesticide a.i.s application to the other due to different emissions fractions related to environmental conditions and a.i.s properties.

Huge differences were found between the two static approaches (Ecoinvent and Neto et al. 2012) and PestLCI 2.0 based emission quantification and FwEtox, The static approaches over-evaluate emissions and hence FwEtox from 2 to 31 times compared to PestLCI 2.0, due to different technosphere/ecosphere boundaries and accounting of degradation and plant uptake phenomena by PestLCI 2.0.

Some of the new PestLCI model parameters can also be used for other perennial or bush crops as long as equipment, shape of the canopy and pesticides a.i.s stay in the range of available options.

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