Set of improved and documented pesticide emission models for use in LCA and guidance on fate modelling

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1. Introduction

Modeling emission is crucial but also comes with challenges. The present deliverable provides an overview of how pesticides are currently addressed in emission inventory. Additional aspects are discussed including the relevance of spatiotemporal variability in modeling emission.

The present deliverable gives an overview of existing data and modeling approaches relevant for addressing pesticides in environmental assessments. Special focus is set on pesticide application and emission quantification, while a more detailed of impact assessment methods is provided elsewhere (see Fantke et al., 2018). The present document thereby constitutes a summary of a more detailed book chapter, where different emission and impact assessment approaches for pesticides are presented in more detail (see Fantke, 2019).

The present deliverable will provide an overview of the state-of-the-art and challenges in emission and impact modeling of agricultural pesticides with the aim to help the reader understanding how pesticides can currently be addressed in environmental assessments, and to find practical information and sources for related data and tools.

2. Pesticide emission models for use in LCA

2.1 Overview of existing emission estimation approaches

Agricultural pesticides generally affect in a negative way the environment along their life cycle. Only recently, quantitative and mass balance based approaches have become available in this context to consistently quantifying pesticide field emissions and associated exposures and impacts on ecosystem quality and human health (Rosenbaum et al., 2015; Fantke et al., 2017). However, despite these approaches, there are still several gaps and unresolved questions in the environmental assessment practice, specifically in the life cycle inventory (LCI) and life cycle impact assessment (LCIA) phases of LCA for agricultural pesticides. Due to these gaps and questions, the field of addressing pesticides in LCA is continuously being advanced by researchers, modelers, and practitioners.

Since emissions are usually not known, they have to be estimated or modeled. Pesticide emissions are usually estimated based on applied pesticide mass, and various statistics exist to derive applied pesticide mass. Detailed information on the actually applied amount of specific pesticides to a particular crop usually requires the access to regulatory reports. However, these reports can inform about which amount of pesticides should be applied per application, but do not contain information on when and where it is actually applied, since this depends on the incidence of pests and diseases, farming systems and practice, etc.

Summary statistics across target or chemical classes at the global scale is provided by the Food and Agricultural Organization (FAO) Corporate Statistical Database (FAOSTAT) in their global pesticide use trends (http://fao.org/faostat). However, these data should be interpreted with great care, because these use statistics are not comprehensive and often aggregate data at different levels.
For modelling pesticide emissions for environmental assessments, one of the most relevant information is the amount of pesticides used related to the given functional unit. As for agricultural pesticides, the amount of pesticides used typically relates to the overall pesticide mass applied on a crop either as field or greenhouse application for a given treated area.

For quantifying emissions from agricultural pesticides applied to field or greenhouse crops, different approaches are available and have been followed by practitioners. These approaches range from assuming fixed emission fractions to particular environmental compartments across all pesticides and crops to mass balance based models distinguishing emission fractions as function of pesticide properties, crop characteristics, environmental conditions, and application scenarios. A review of various pesticide emission models is provided in Mottes et al. (2014). In LCA, one of the most widely applied assumption for pesticide emission fractions is that 100% of the applied mass is emitted to soil (within the agricultural field), thereby considering the field soil as part of the ecosphere. Other approaches are available, differentiating emissions into more than a single environmental compartment, such as 75% emitted to field soil and 25% to air for viticulture crops (Neto et al., 2013) or 96% emitted to air and 4% to surface water outside the field (USDE United States Department of Energy, 2012). Table 1 provides an overview of the different available emission estimation approaches currently applied in LCA and other environmental assessments of pesticides.

Table 1: Distribution of pesticide emissions after application to crop in selected LCI databases.
(Adapted from Fantke 2019)

<table>
<thead>
<tr>
<th>Emission fraction to:</th>
<th>Approach 1</th>
<th>Approach 2</th>
<th>Approach 3</th>
<th>Approach 4</th>
<th>Approach 5</th>
<th>Approach 6</th>
<th>Approach 7</th>
<th>Approach 8</th>
</tr>
</thead>
<tbody>
<tr>
<td>Field</td>
<td>Ecoinvent2</td>
<td>Neto et al.2</td>
<td>U.S. LCI3</td>
<td>USDA Ag-LCI4</td>
<td>JALCA5</td>
<td>WFDB6</td>
<td>AgriBalyse MEANS</td>
<td>AgriFootprint PestLCI PestLCI Consensus</td>
</tr>
<tr>
<td>Agricultural soil</td>
<td>100%</td>
<td>75%</td>
<td>-</td>
<td>100%</td>
<td>100%</td>
<td>100%</td>
<td>90%</td>
<td>var.12</td>
</tr>
<tr>
<td>Crops</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>var.12</td>
</tr>
<tr>
<td>Air</td>
<td>-</td>
<td>25%</td>
<td>~95%10</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>9% var.</td>
</tr>
<tr>
<td>Agricultural soil</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>var.</td>
</tr>
<tr>
<td>Natural soil</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>var.</td>
</tr>
<tr>
<td>Surface water</td>
<td>-</td>
<td>-</td>
<td>~5%11</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>1% var.</td>
</tr>
<tr>
<td>Groundwater</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>var.13</td>
</tr>
<tr>
<td>Other8</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>var.12</td>
</tr>
</tbody>
</table>

*Off-field area requires to apply an area distribution as described in the subsequent paragraph.
1 Ecoinvent database until version 3.4 (Nemecek and Kägi, 2007; Nemecek and Schnetzer, 2011)
2 Fixed emission fractions specifically estimated for viticulture (Neto et al., 2013)
3 U.S. Life Cycle Inventory database (USDE United States Department of Energy, 2012)
U.S. Department of Agriculture Commons Life Cycle Inventory datasets (Cooper, 2015)
National Agriculture and Food Research Organization, Japan LCA database (Hayashi et al., 2012)
World Food LCA Database until version 3.3 (Nemecek et al., 2015)
PestLCI model version 2.0; point emissions over distance range to field edge (Dijkman et al., 2012)
Adapted and further developed from PestLCI 2.0; area-integrated emissions over distance range to field edge (Rosenbaum et al., 2015; Fantke et al., 2017)
Processes leading to a reduction of emission fractions to the environment, e.g. degradation and plant uptake
Emissions modeled as function of pesticide vapor pressure, but typically little deviation from values ~95% (US-EPA United States - Environmental Protection Agency, 1995)
Emissions modeled as function of pesticide and soil properties, but typically little deviation from values ~5% (Kellogg et al., 2002)
Any fraction not used as input for subsequent impact characterization (e.g. degradation fraction)
Currently, no matching characterization factors for groundwater emissions in any available LCIA method

An alternative to assuming fixed emission fractions is proposed by modeling the initial distribution of pesticides on the agricultural field and subsequently estimating emissions into different environmental compartments. A model that follows this approach is PestLCI (Hauschild, 2000; Birkved and Hauschild, 2006). PestLCI was adapted based on a global consensus building effort. Focus in this effort was on (a) defining the boundary between emission inventory and impact assessment for pesticides in LCA, and (b) adapting PestLCI 2.0 (Dijkman et al., 2012) to better meet the needs for LCA, such as integrating emissions over the entire relevant area (instead of estimating point emissions) and defining a consistent set of global crop, application, climate, and soil archetypes. Additional, parallel efforts around improving and expanding PestLCI focused on adapting the model for viticulture (Renaud-Gentié et al., 2015) and for tropical conditions (Gentil et al., 2019).

Outcomes of the overall consensus building process are among other an improved emission model (namely “PestLCI Consensus”) that comes with a suite of improved drift functions, and a flexible approach to addressing field soil as part of the environment (Fantke et al., 2017). Varying emission fractions are thereby referring to modeled output that differs between combinations of pesticides, crops, and application scenarios (e.g. climate, soil type, application method).

Emissions that reach off-field areas would have to be allocated to the respective compartments according to an area distribution. The involved compartments should match those compartments that are used in impact assessment models, such as USEtox. In the case of USEtox, off-field emissions would have to be allocated according to the area distribution in a given region between agricultural soil, natural soil and freshwater. If other compartments are relevant in a given region (e.g. forest, urban areas, industrial soil), these areas would have to either be allocated to any of the available compartments used in the LCIA model applied as otherwise any related emission would be ignored in the related impact characterization.

However, there is currently no consensus on which geographical scope we should take as reference for distributing off-field areas according to the related LCIA model compartments. There is furthermore no consensus on using either fixed area distribution fractions or using GIS-based tools for each specific emission scenario. One possible approach would be to apply fixed area distribution fractions for background processes, e.g. aligned with the geographical scope of...
respective LCIA model or according to the geographical scope of the LCA if not global. For foreground processes, in contrast, more localized and GIS-based area distributions could be applied, aligned with the geographical scope of these foreground processes in each LCA study.

2.2 Recommended emission estimation approach

We follow the general recommendations provided in Rosenbaum et al. (2015) for modelling environmental emissions of pesticides in LCA by recommending to use the PestLCI Consensus model that has been implemented as a web-tool under the auspices of the OLCA-Pest project and which is available under [https://pestlciweb.man.dtu.dk](https://pestlciweb.man.dtu.dk).

The following main improvements have been implemented in the PestLCI Consensus model as compared to PestLCI 2.0:

Primary distribution fraction processes:
- Distribution within **first minutes** after application
- Distribution in air (emission), field crop leaf surfaces, field soil surface, and off-field surfaces (emission), of which the latter two include cover crop surfaces in cases where respective buffer zone are defined

Secondary emission fraction processes:
- Fate and distribution within a **user-defined time period** after application
- Soil volumetric water content assumed to equal calculated field capacity
- Degradation in crops based on dissipation half-life as proxy (as used in USEtox 2.0x)

Details on the individual improvements are provided in Table 2.

Table 2. Improvements of the PestLCI Consensus web-tool compared to PestLCI 2.0.

<table>
<thead>
<tr>
<th>Modifications</th>
<th>PestLCI 2.0</th>
<th>PestLCI Consensus model</th>
</tr>
</thead>
<tbody>
<tr>
<td>Calculation of volatilization from soil</td>
<td>Fugacity model, using molecular volume to calculate diffusivity of pesticide</td>
<td>Fugacity model, using molar mass to calculate diffusivity of pesticide with adapted parameterizations</td>
</tr>
<tr>
<td>Calculation of pesticide uptake in leaves</td>
<td>Log k(lu) calculation depending on leaf type</td>
<td>Uptake into crops via leaves based on pathway through cuticle (based on processes also implemented in dynamiCROP)</td>
</tr>
<tr>
<td>Calculation of volatilization from leaves</td>
<td>Regression kvolatilization=f(VP)</td>
<td>Volatilization from leaves based on flux through air</td>
</tr>
</tbody>
</table>
### 3. Guidance for environmental fate modelling

#### 3.1 Existing fate modelling approaches

Emissions modeled in the PestLCI Consensus framework are presented at two different levels. The first level covers initial deposition processes of the pesticide formulation during the first minutes after pesticide application. Output of this level are so-called “initial distribution fractions”, also called “primary distribution fractions”. The second level goes beyond the first minutes after pesticide application and includes processes occurring at the field and beyond the field over a period of e.g. 1 day or 1 week. These processes include volatilization from crop and soil surfaces, leaching through the soil column and sub-surface runoff, are essentially modeled as first order processes and also covered in the environmental fate modelling component of life cycle impact assessment (LCIA) models, such as USEtox (Rosenbaum et al., 2008). Output of the second level are so-called “secondary emission fractions”, since these consider initial (or primary) and secondary (i.e. follow-up) processes for deriving emission fractions. Reasons for including these fate processes in LCI modelling while they are already covered in LCIA models as part of steady-state fate solutions is to achieve a more realistic emission distribution that is connected to the respective characterization factors.
Ecotoxicity impacts associated with environmental emissions of agricultural pesticides can generally be characterized the same way as impacts from non-point emissions of other chemical substances. The ecotoxicity impact pathway for agricultural pesticides thereby follows the general impact characterization framework combining environmental fate, ecosystem exposure, and ecotoxicity effects as implemented in different impact characterization models including USEtox (Rosenbaum et al., 2008; Henderson et al., 2011), Impact2002 (Pennington et al., 2005), CalTOX (McKone and Enoch, 2002), and USES-LCA (van Zelm et al., 2009). An overview of how environmental fate processes as part of LCIA are modeled is provided in Henderson et al. (2011), Fantke et al. (2018) and Fantke (2019). Additional details for how to address the modelling of environmental fate processes specifically for pesticides are provided in OLCA-Pest Deliverable D4.2.

3.2 Spatiotemporal variability

For the quantification of pesticide emissions, at least during the field application, some degree of spatial differentiation is currently possible by using data on specific climate and soil regions (Dijkman et al., 2012; Fantke et al., 2017). For initial distribution fractions, the consideration of spatial aspects is generally limited to the occurrence of crops, related application methods, the field width and the occurrence of buffer zones. For secondary emission fractions, the options for considering spatial aspects, such as differences in soil and climate conditions, field characteristics and application aspects (e.g. buffer zones) can be included, where such data are available to practitioners.

Also in the impact assessment of agricultural pesticides, a regionalized assessment, i.e. considering geographical differences, is generally relevant, for example by using tropical species in the ecotoxicity effect assessment of agricultural pesticides in tropical regions.

Overall, spatial variability can be the dominant driver of differences in emission and impact results. Given the large spatial variability of emissions and related impacts, spatialized models should hence be used whenever emission locations are known. If emission locations are unknown, it is recommended using archetypes to represent aspects that drive variabilities in assessment results, such as field size, crop, and environmental conditions.

Since it is currently unclear what specific timeframe is covered in the initial (primary) distribution fractions, a related definition could be proposed where initial distribution fractions consider just the (nearly) immediate distribution processes that happen directly after pesticide application. With that, initial distribution fractions would miss potential subsequent processes occurring several hours after pesticide application.

However, the temporal dynamics, the selection of related pesticides and application methods might vary by crop and location (Yang and Suh, 2015) and these aspects are important to determine which emission distribution processes to consider in the emission inventory analysis (Rosenbaum et al., 2015). This can on the one hand just be to consider the (nearly) immediate distribution of the applied pesticide formulation within the first minutes after application, where usually only initial deposition and wind drift are relevant. On the other hand, this could also be extended to consider all subsequent processes when including several hours to days after
application, e.g. subsurface runoff, leaching and preferential flow through the soil column, plant uptake through leaves and roots, re-emission and volatilization from soil, water and plant surfaces. For processes like deposition onto field soil, first-order processes are usually modeled, while wind drift requires an integration over the relevant time, which is reflected in the drift functions that are implemented in currently used emission inventory models for pesticides (Dijkman et al., 2012; Fantke et al., 2017).

When applying initial distribution fractions would mean that there is a potential risk not to account for some relevant emissions that are characterized, we propose to use secondary emission distribution fractions specifically for those studies that have a specially focus on pesticides emissions and related impacts in the foreground system.

References


Nemecek, T., Kägi, T., 2007. Life cycle inventories of Swiss and European agricultural production systems; Final report ecoinvent v2.0 No. 15. Swiss Centre for Life Cycle Inventories, Duebendorf, Switzerland, p. 360.

Nemecek, T., Schnetzer, J., 2011. Methods of assessment of direct field emissions for LCIs of agricultural production systems. Swiss Centre for Life Cycle Inventories, Duebendorf, Switzerland, p. 34.


