SETAC

Spatially Distributed Leaching Modelling of Pesticides in the context of Regulation (EC) 1107/2009

Problem definition document

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Abstract

Spatially distributed leaching modelling (SDLM) of pesticides is a methodology to estimate the leaching potential of plant protection products over an extensive spatial scale such as national or European. It is described as a higher tier in the current European Guidance for groundwater risk assessment. Whereas this option is an integral part of the tiered assessment scheme only little guidance is provided on how to conduct such spatial assessments with SDLM. Guidance on how to perform such leaching assessments is therefore needed, as well as version control for high-resolution spatial databases for the EU. It was therefore decided to establish a working group under the umbrella of the SETAC Environmental Monitoring Advisory Group on Pesticides (SETAC EMAG-PEST). This document describes the aim and scope of the work to be performed by this working group.

The main products of the working group will be a harmonised modelling framework including the data needed to run these models, and documents describing the use of the framework in regulatory assessments. The framework will serve two different Tiers of the groundwater risk assessment scheme, i.e. Tier-3b and Tier-4. At Tier-3b, the framework will deliver the same exposure assessment goal as currently used in FOCUS groundwater, i.e. the 80^{th}-spatial and temporal percentiles of the leaching concentration at 1-m depth. This exposure assessment goal is considered a conservative estimate of the real groundwater concentration. To ensure consistency of the tiered approach, the modelling framework will support all parameter refinements carried out at Tier-2. At Tier-4, the measured groundwater concentration in groundwater wells is assessed. The modelling framework plays a crucial role for the selection of vulnerable regions in which to install monitoring wells. It can also be used to demonstrate whether existing groundwater monitoring studies have been carried out at locations that are sufficiently vulnerable in view of the existing FOCUS exposure assessment goal. The modelling framework will, however, not simulate the actual concentration in the groundwater wells, because additional processes occur between 1-m depth and the position of the groundwater wells.

The Working Group will consist of member from academia, regulators and industry. It will consist of a Steering Committee, a subgroup on spatial data and a subgroup on modelling. The Working Group will deliver two years after the start of the project.

Preface

Spatially distributed leaching modelling (SDLM) of pesticides is a methodology to estimate leaching potential over an extensive spatial scale such as national or European. It is described in the current European Guidance for groundwater risk assessment (EC 2014) and foreseen to be used as higher tier leaching risk assessment on Tier-3b as well as supporting monitoring studies (Tier 4). In the resolutions of the 9th European Modelling Workshop 2018 (http://www.pfmodels.org/emw9.html) it was agreed that a dialog on a spatial modelling framework is needed as well as version control for high-resolution spatial databases for the EU. Also in the recent publication of a previous SETAC EMAG-Pest GW working group on groundwater monitoring studies, it has been shown that Spatially Distributed Leaching Modelling (SDLM) is of great importance for performing spatial vulnerability assessment regarding leaching of pesticides to groundwater and to identify vulnerable sites within an area of interest for groundwater monitoring (Gimsing et al. 2019).

A group of interested scientists decided to organise a workshop on SDLM, bringing together international experts in GIS and groundwater modelling from academia, regulatory authorities, research institutes, contract organisations and industry. A first workshop on SDLM was held on 24 May 2019 in Ghent, Belgium, where it was agreed that a harmonised framework on SDLM would be valuable and should be developed. It was proposed that SETAC would be a good platform for the development of a harmonised framework for SDLM, since restrictions of resources were seen with EFSA and Member States. A follow-up meeting was held between the participants of the workshop and members of the former SETAC EMAG-Pest GW group prior to the Pesticide Symposium in Piacenza 2019. In the meeting it was confirmed that SETAC would be the appropriate platform for a working group for the development of a harmonised framework for SDLM, and that a steering committee should be formed. The tasks of this steering committee should be to define the scope of the working group, and subsequently setup a functioning working group.

In the fall of 2019, a Steering Committee was formed from the organisers of the initial workshop in Ghent, supplemented with representatives of regulatory authorities from all three regulatory zones in Europe. SETAC agreed to host the initiative under the SETAC Environmental Monitoring Advisory Group on Pesticides (EMAG-Pest), and officially formalised the Steering Committee at the SETAC Europe Online meeting in May 2020. First product of the Steering Committee is this problem definition document, describing the aim and scope of the work to be performed by the working group.

The Steering Committee would like to thank Mark Egsmose (EFSA; member of the SETAC Europe Council) for establishing the first communication with SETAC, and Anne Alix, chair of the SETAC Environmental Monitoring Advisory Group, for the opportunity to form a working group under the umbrella of the Advisory Group. The Steering Committee would also like to thank JRC Joint Research Centre for their support in hosting the SDLM-website https://esdac.jrc.ec.europa.eu/projects/sdlm.

Contents

1 Introduction

1.1 Background to the development of a guidance document on SDLM

The initiative to develop a harmonised guidance on Spatially Distributed Leaching Modelling (SDLM) was started after the 9th European Modelling Workshop in 2018 in Copenhagen where in the resolutions it was concluded that a dialog is needed on a Spatially Distributed Leaching Modelling Framework for[1]:

- selecting appropriate monitoring sites;
- setting existing sites into context.

It was further concluded that:

- requirements are needed on input and output of appropriate spatially-distributed models;
- version control is needed for high-resolution spatial databases for the EU.

SDLM is listed as one of the higher tier options (e.g. Tier-3b) for leaching assessment on European, zonal or member state regulatory level in the FOCUSgw higher tier report (Figure 1; EC 2014). Whereas this option is an integral part of the tiered assessment scheme only little guidance is provided on how to conduct such spatial assessments with SDLM. However, on national level there are examples where this is already implemented (GeoPEARL in the Netherlands, Van der Linden et al. 2004; Frogs in France, Beigel et al. 2013; MACRO_SE in Sweden, Boström et al. 2015), and thus SDLM shows the practical relevance.

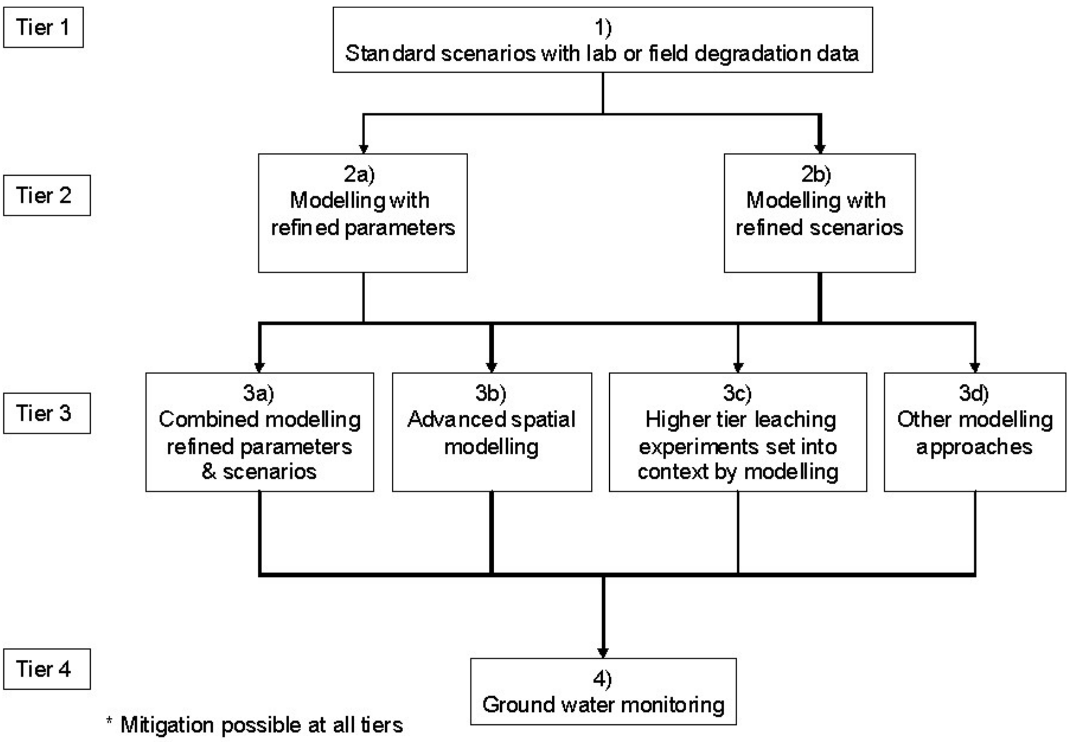

Figure 1: Tiered assessment scheme of FOCUSgw (EC 2014)

Also, in the report of a previous SETAC EMAG-Pest working group on groundwater monitoring studies, it has been shown that Spatially Distributed Leaching Modelling (SDLM) is of great importance for performing spatial vulnerability assessment regarding leaching of pesticides to

[1] http://www.igordubus.com/pfmodels/EMW9_resolutions.pdf

groundwater and to identify vulnerable sites within an area of interest for groundwater monitoring. Examples for SDLM are already included in this report (Gimsing et al. 2019).

Although there are versions of spatially distributed models available at the scale of the EU (Tiktak et al. 2002; Tiktak 2012; Hoogeweg et al. 2015; 2018), it can be stated that currently no harmonised framework exists on how to conduct SDLM. Different methods based on different geodata sets and models are currently submitted by applicants in dossiers for active substance approval or product registration, resulting in a lack of regulatory acceptance. There is also a need to ensure the quality of the data sets (e.g. by means of version control) as well as to improve the reproducibility and transparency of the methods used in such an approach.

1.2 Benefits of the SDLM-initiative

Spatially Distributed Leaching Modelling is a method that allows the movement of a substance through soil, and thereby potentially into groundwater, to be quantified. The current state of computing power is such that it is now possible to quantify this potential by means of modelling across the entire agricultural landscape of the EU (Tiktak et al. 2004; Hoogeweg et al. 2018; Beigel et al. 2013). Modelling provides a consistent and unbiased way of quantifying leaching potential and comparing estimates of this potential between locations across the whole of a potential use area.

Spatially distributed leaching modelling of plant protection products has been conducted for nearly 25 years (Corwin et al. 1996; Tiktak et al. 1996). As soon as it became practical to link models with a Geographic Information System (GIS) or embed within a GIS, regulators, academia and industry have been using SDLM. The two main benefits of spatially distributed modelling for regulatory use are:

- that it is possible to model any landscape from field-level to an entire continent in a consistent manner;
- that it is possible to rank areas or locations with respect to leaching vulnerability[2].

With respect to the first benefit, spatially distributed modelling offers the advantage that exposure patterns are predicted for each time and location of the area of interest for a certain pesticide use. This makes it possible to select the exact time-space combination of the area of interest that is in accordance to the pre-defined exposure assessment goal. Spatial aspects of the area of interest such as application to a certain crop or in a certain region may be considered.

The second benefit of spatial modelling – ranking of areas or locations – is of critical importance for the interpretation of groundwater monitoring studies. An important question is whether existing or dedicated groundwater monitoring locations can be considered sufficiently vulnerable to groundwater leaching in accordance with the pre-defined exposure assessment goal. This can be achieved by comparing the leaching vulnerability of monitoring sites with the time-space concentration of the entire area of interest (*in context setting of monitoring sites*). For the design of groundwater monitoring studies, it can be used to rank sites and/or regions regarding their vulnerability against each other and select locations that can be considered as sufficiently vulnerable in accordance with the pre-defined exposure assessment goal.

An additional benefit of spatially distributed assessments is that it can be used to develop targeted mitigation measures for a certain pesticide use and to check and demonstrate the potential effectiveness of this measure.

This SDLM-initiative is aimed at groundwater leaching. It can, however, also be regarded as a precursor for developing a harmonised framework on spatially distributed modelling concerning other compartments such as soil or surface water, which might be used in combination with

[2] Gimsing et al. (2019) distinguish between site/soil vulnerability, or leaching vulnerability and aquifer vulnerability. Spatially distributed modelling developed so far is primarily aimed at leaching vulnerability.

spatially distributed ecotoxicological assessments in future (e.g. EFSA PPR Panel 2015; Topping et al. 2015).

1.3 Scope and structure of the SDLM working group

A working group is started under the umbrella of SETAC. The scope of the working group is to a) develop a harmonised framework for conducting spatially distributed leaching modelling at the European or zonal level and b) to provide documents that describe the framework and its elements as well as its use for regulatory purposes.

In a first step, such an approach should be focused onto the European scale. However, the methodology should also allow conducting leaching assessments on zonal, member state or even regional level if spatial and temporal data are considered appropriate.

The working group will consist of a steering group and two subgroups.

- The **steering group** is responsible for the problem formulation, organisation of the project, communication with risk managers and the final report. The steering group also has the task to discuss the regulatory aspects of the project since it was decided not to have a separate subgroup on regulatory aspects. The problem formulation includes the (provisional) formulation of the exposure assessment goal (see Chapter 2). It is the intention of the steering group to publish the final report in a peer-reviewed journal. The steering group consists of members from academia, authorities, contract research organisations (CRO’s) and industry. The steering group is chaired by Anton Poot (Ctgb, the Netherlands) and co-chaired by Aaldrik Tiktak (PBL Netherlands Environmental Assessment Agency, the Netherlands) and Bernhard Jene (BASF SE, Germany). Further details on regulatory aspects are provided in Chapter 2.
- The **geodata subgroup**, which should make recommendations about the geodata and temporal data to be used for SDLM depending on the spatial scale. This includes crop, land use/cover, soil and geohydrological data. Additionally, temporally relevant data such as daily weather data, cropping data, management practices will be included as well. An inventory and review of existing databases needs to be performed. Version control within or outside the FOCUS version control group needs to be promoted and supported. Data holders need to be taken on board of the discussion and as needed define what the main purpose of the dataset is, its quality control, gaps, improvement needed and maintenance. Further details on the geodata subgroup are described in Chapter 3.
- The **modelling framework subgroup**. This subgroup needs to make recommendations of the models and tools that are seen appropriate to be used for SDLM. The focus should be on models which are already used for (lower tier) leaching assessments in the current EU registration procedure and for which also experience exists with spatially based approaches (e.g. it should be feasible to run the model for a continental/sub-continental level). For this initial phase of the SDLM project, modelling will be focused on the vertical downward transport through the (mostly) unsaturated soil zone. Further details are in Chapter 4.

1.4 Overview of this document

Chapter 2 describes the regulatory boundary conditions for the SDLM-framework. This includes the exposure-assessment goal and the boundary condition to ensure consistency of the tiered approach. Chapter 3 describes available databases for spatially distributed modelling and describes the most important quality requirements. Chapter 4 describes the available software tools and requirements for these tool(s). Chapter 5 provides some overall conclusions and discussion points.

2 Regulatory boundary conditions

In the Ghent workshop and follow-up meeting of this initiative several regulatory boundary conditions were discussed. These boundary conditions are detailed in this chapter. This includes the position of SDLM in the tiered approach (Section 2.2) and the definition of the exposure assessment goal (Section 2.3). Gimsing et al. (2019) concluded that exposure assessment goals (also called specific protection goals) are a central issue regarding the evaluation of groundwater leaching. However, it is beyond the scope and the competence of the SDLM-working group to define specific groundwater protection goals since for this political and socio-economic aspects need to be considered. Nevertheless, discussions should take place how different exposure assessment goals can be addressed with SDLM.

2.1 Scope and limitations of the framework

As described in Section 1.1, the SDLM-framework[3] should contribute to the harmonised leaching assessment of plant protection products and its metabolites in the EU. So the framework should support the FOCUS tiered approach as described in Figure 1 by simulating the spatiotemporal distribution of the annual, biennial or triennial average leaching concentration of a substance and its metabolites at 1-m depth in the area of use in each of the nine FOCUS climatic zones. More specifically it should calculate from this distribution the exposure assessment goal at **Tier-3b** as realistically as possible (see section 2.2 for the exposure assessment goal in FOCUS 2009). The above implies that at Tier-3b the SDLM provides an endpoint that is completely in line with the endpoint simulated at Tier-1 and Tier-2.

For **Tier-4** SDLM should calculate the relative vulnerability of the upper soil layer (until 1-m depth) for selecting vulnerable sites or areas for designing a groundwater monitoring network and for in context setting of existing monitoring sites. Therefore, a different endpoint is assessed, i.e. the measured concentration in the monitoring well. Additional processes occur between 1-m depth and the position of the groundwater wells. These processes are not accounted for in the currently proposed version of the SDLM. As described in Gimsing et al. (2019) additional work is needed, for example to demonstrate the connectivity of treated fields at the soil surface and the groundwater well. This work is outside the scope of this Working Group.

The framework should be ready-to-use for the above purposes, which means that both the software and appropriate data need to be included. The framework should also be applicable for higher tier leaching assessments of plant protection products at the national level in EU Member States in accordance with Regulation (EC) No. 1107/2009. However, since most Member States have more detailed soil, climate, and crop data available, the software must be able to include these more detailed datasets.

2.2 Ensuring consistency of the tiered approach

As indicated in Figure 1, SDLM is a higher tier approach, so the 90th-percentile concentration derived from SDLM should be a less conservative estimate of the groundwater concentration than Tier-1 and Tier-2. To ensure this, it is first necessary that the framework can handle all parameter refinements that have been introduced at Tier-2, including for example aged sorption and pH-dependent sorption. If this is not done, spatially distributed modelling at Tier-3b could give higher concentrations than modelling with refined parameters at Tier-2a. Inconsistencies can also result because Tier-1 and Tier-2a consider the entire agricultural area within a FOCUS zone, whereas at Tier-3b the area where the intended crop is grown is the area of interest. Whether Tier-3b delivers indeed lower concentrations than Tier-1 and Tier-2, can only be demonstrated after an agreed version of the SDLM-tool has been made available. To ensure consistency of the tiered approach, calibration of Tier-1 and Tier-2 might be necessary (see EFSA 2017 for examples). This work is,

[3] The SDLM-framework consists of models including the data needed to run these models. The framework can consist of multiple models with the same purpose that are, however, harmonised.

however, outside the scope of the Working Group because it would imply an implicit change of Tier-1 and Tier-2.

Another requirement of tiered approaches is that the higher tiers should give a more realistic estimate of the groundwater concentration. Here, we consider three important processes that might influence the conservativeness of Tier-3b, i.e. (i) losses by drainage, surface runoff and interflow, (ii) the occurrence of preferential flow, and (iii) canopy processes.

Lateral flow processes
The FOCUS models are purely one-dimensional models, which means that several loss processes such as runoff, interflow and subsurface (artificial) drainage are not included. This is not a real issue for Tier-1 leaching assessments, because these scenarios should represent worst-case conditions and because of this these processes are ignored in Tier-1 assessments (EC 2014). In a higher-tier spatially distributed leaching assessment, however, ignoring these processes may lead to incorrect prediction of spatial patterns of leaching vulnerability. Sites might be indicated as highly vulnerable even if most of the incoming precipitation and applied substance is lost to surface water via horizontal flow processes. In order to get a realistic spatial description of the vulnerability and for obtaining realistic leachate concentrations, it is essential to also consider lateral flow processes to surface waters. Incorporation of runoff processes could make the modelling much more complicated, so a compromise between model detail and applicability needs to be found here. However, this compromise should be scientifically justified.

Preferential flow
Another process that is ignored in Tier-1 and Tier-2 groundwater leaching assessments is the occurrence of preferential flow. The only exception is the Châteaudun scenario, where the MACRO model has been parameterised to show the impact of preferential flow but the role of this scenario for decision making is not clear. There is consensus that this process is important for correctly describing the transport of pesticides through structured soils; however, there is currently no harmonised method available to derive the parameters needed for describing preferential flow at the regional scale. Ignoring preferential flow may lead to underestimation of the leaching fluxes and incorrect prediction of spatial patterns of leaching vulnerability, particularly if part of the study area consists of structured soils or – more extremely – karstic soils[4].

Introduction of preferential flow at Tier-3b would make the assessment more realistic; however, because the process is not (yet) systematically included at Tier-1 and Tier-2, introduction of preferential flow at Tier-3b could lead to inconsistencies of the tiered approach. This can only be repaired if the Tier-1 and Tier-2 FOCUS scenarios would be revised. Given all these problems, the SDLM-framework will for the moment not include the simulation of pesticide leaching by preferential flow. If an agreed methodology for assessing preferential flow would become available, this could be introduced in the SDLM-framework, but this is only meaningful if at the same time also the FOCUS groundwater scenarios at Tier-1 and Tier-2 are revised. During such a revision, recent developments should be taken into account (e.g. with respect to crop interception, wash-off and aged sorption).

Canopy processes
At Tier-1 and Tier-2, interception of pesticides by the crop canopy can be simulated. Since the introduction of the FOCUS groundwater scenarios, it has been common practice to reduce the application rate by the fraction that is intercepted by the crop canopy and to apply this reduced fraction to the soil (EC 2014). As described by EFSA PPR Panel (2010), this approach is not considered defensible because there is insufficient evidence that wash-off from the crop canopy can be ignored. For this reason, EFSA (2015) recommends including the effect of dissipation at the crop canopy and foliar wash-off when the substance is applied to the crop canopy.

Addition of foliar wash-off and dissipation at Tier-3b would make the assessment more realistic but potentially also more conservative. It is envisioned that the Tier-1 and Tier-2 scenarios will be

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[4] A karst landscape is a landscape topography formed from the dissolution of soluble rocks such as limestone, dolomite, and gypsum, and characterised by underground drainage systems with sinkholes and caves.

revised to include these processes in the future. The Working Group therefore proposes to include these processes as an option into the SDLM-framework; however, it is not recommended to include these processes in regulatory assessments as long as Tier-1 and Tier-2 have not been revised.

2.3 The provisional exposure-assessment goal

Exposure-assessment goal provisionally based on FOCUS (2009)
Development of a scientific methodology for the assessment of leaching into the groundwater requires an exact definition of the exposure-assessment goal (EFSA 2010; 2012)[5]. This exposure-assessment goal describes which groundwater needs to be protected and over what time period. This is a risk-management decision. Gimsing at al. (2019) describe seven options for exposure-assessment goals ranging from extremely conservative to pragmatic. Since there is currently no agreement on the exposure-assessment goal at the European level, the methodology described in this document is provisionally based on the goal to assess the 90^{th}-percentile of the leaching concentration at 1-m depth considering all agricultural fields within a FOCUS climatic zone where the particular product is intended to be used. The agricultural area of use is represented by the crop in which the pesticide is intended to be used, e.g. for a pesticide that is to be applied in maize, the area is defined as all fields growing maize in a FOCUS climatic zone. The 90^{th}-percentile leaching concentration is estimated by the combination of the 80^{th}-temporal percentile of 20 annual average leaching concentrations and the 80^{th}-spatial percentile. This definition is in line with FOCUS (2009) and EC (2014).

An important characteristic of tiered approaches is that the same exposure-assessment goal should be used in all tiers. Furthermore, higher tiers must be more realistic and less conservative. As mentioned above, the proposed exposure assessment goal for Tier-3b is consistent with the exposure-assessment goal for Tier-1 and Tier-2. This exposure-assessment goal, however, does not directly refer to the concentration in the groundwater. Instead, it is assumed implicitly that the leaching concentration at 1-m depth is a **conservative surrogate** for the groundwater concentration – although in certain scenarios, such as Kremsmünster, groundwater is simulated to rise above the assessment depth of 1 meter.

Considerations for risk managers for the final exposure assessment goal
Whether the FOCUS exposure assessment goal is conservative enough to protect (deeper) groundwater aquifers, can only be assessed after risk managers have decided on the final exposure assessment goal for these deeper groundwater aquifers. There are four important quantities to look at: (i) the depth, (ii) the spatial area over which a concentration is averaged, (iii) the time over which a concentration is averaged, and (iv) the spatiotemporal percentile of the exposure assessment goal.

With respect to **depth**, it is likely that deeper depths result in lower concentrations due to e.g. dispersion and/or dissipation/degradation processes. So, if the same spatiotemporal percentile is used, a deeper depth than 1-m would be less conservative than the provisional exposure assessment goal (i.e. the FOCUS approach aiming at 1-m depth), because it will generally deliver lower concentrations than the FOCUS modelling. This approach is taken in the Netherlands. Here, the exposure-assessment goal is the 90^{th}-spatiotemporal percentile of the groundwater concentration at 10-m depth (Van der Linden et al. 2004). It has been demonstrated that the concentration at 10-m depth is generally lower than the concentration at 1-m depth (Tiktak et al. 2005).

Another aspect of the exposure assessment goal is the **area over which the concentration is to be averaged**. The Groundwater Directive states that all groundwater bodies should have a good chemical status by 2027 latest. These groundwater bodies generally cover a larger area, e.g. in the Netherlands there are 23 groundwater bodies. According to the Guidance on groundwater status and trend assessment (EC 2009), good chemical status is reached if <u>all monitoring points</u> within these groundwater bodies comply, or only a certain percentage of monitoring wells exceeds the

[5] EFSA PPR Panel (2010) uses the word Specific Protection Goal for ecotoxicological endpoints. Gimsing et al. (2019) used the word Exposure Assessment Goal for the exposure assessment. Exposure Assessment Goals and Specific Protection Goals can be used as synonyms.

groundwater concentration quality standards (the proposed default value by the Commission is 20%) but appropriate investigations confirm that there is no deterioration in quality of waters for human consumption. The consequence is that even though the Groundwater Directive aims at larger water bodies, spatial averaging of concentrations is not performed. However, the Groundwater Directive allows for **temporal averaging** because testing against regulatory thresholds is done against "annual arithmetic mean concentrations", which are calculated as the mean of all the annual average concentrations of a monitoring site for a six-years period. Using annual mean concentrations is in line with the FOCUS approach.

If risk managers would decide to change the **spatiotemporal percentile** to a higher number, it can no longer be guaranteed that the FOCUS approach is protective enough. For example, the 99th-spatiotemporal percentile at 10-m depth could be more conservative than the 90th-spatiotemporal percentile at 1-m depth. Notice that taking the 99th-spatiotemporal percentile means that all of the monitoring points except 1% should always comply. This is a very conservative assumption, particularly if spatial or temporal averaging is not allowed for as well.

After risk managers have chosen an exposure assessment goal for groundwater, the SDLM-framework could be used to check if the FOCUS exposure assessment goal is conservative enough and appropriate assessment factors could be introduced, if needed (see e.g. EFSA 2017; Van den Berg et al. 2019).

2.4 Cropping and application systems covered by the framework

As indicated in EFSA (2017), there is a huge variety of cropping and application systems (see Figure 2 in EFSA (2017)). EFSA (2017) makes a distinction between annual crops and permanent crops, because the soil in annual crops is usually tilled. It is also important if the crop is planted in rows or whether it covers the entire field. Because this affects the fate of the compound in soil, the framework should be able to handle these differences in an appropriate manner. Another important distinction is based on the application system (sprayed to the soil surface, sprayed to the crop, incorporated). The framework should be able to deal with the different cropping systems and application systems described in Section 1.3 of EFSA (2017); however, the actual datasets may need an update (Chapter 3). Notice that covered crops and rice paddies will not be covered by the framework. The SDLM-framework is furthermore aimed at professional agricultural uses and cannot simulate leaching resulting from point sources such as farm yards and hardened surfaces.

2.5 Interpretation of groundwater monitoring studies (Tier-4)

The SDLM-framework will not be used to simulate the final endpoint at Tier-4, because this endpoint is based on direct measurements of the groundwater concentration. The framework will, however, play an important role in context setting of existing monitoring sites (Gimsing et al. 2019). In this respect, it is important that the SDLM-framework delivers appropriate maps of the relative vulnerability of locations. There are a couple of issues that need to be addressed.

Difference in depth

First, the SDLM-framework delivers the leaching concentration at 1-m depth and not the concentration at the depth of the groundwater wells. It cannot be guaranteed that groundwater recharged under a field treated with a plant protection product, is connected to the groundwater well. Furthermore, the travel time to the groundwater may be longer than the actual use of a product, which means that the well would be unsuitable to demonstrate a safe use. This all means that additional work needs to be done for the interpretation of groundwater monitoring studies (see Gimsing et al. 2019 for more information). Not all of this work will be covered in the SDLM-document.

Mass fluxes instead of concentration for vulnerability assessment

The second issue or problem is that high annual leachate concentrations can be associated with minimal substance mass fluxes if the water volume flux is minimal. Since mixing of these very low mass fluxes in the upper few centimetres of the groundwater already led to a huge decrease in the concentration it can be assumed that leachate concentrations that are associated with a relevant volume flux are of higher importance for the groundwater quality. Similarly, the selection of sites in statistical monitoring studies may require an aggregation of potential leachate to a larger scale. Mass fluxes can be meaningfully added or averaged whereas it is more difficult to do this with concentrations. Since this issue was already seen in Gimsing et al. 2019, they recommend using the annual substance mass fluxes as characteristics for vulnerability in the context of monitoring studies. The consequences of these differences need to be addressed in the final SDLM-documentation.

2.6 Regulatory requirements for geodata

A SDLM framework relies on a wide variety of data sources. Although many data sources are readily available, they may not be suitable for use within a distributed modelling framework due to being incomplete, out of date, or not publicly available. For datasets to be included in the SDLM guidance, a series of criteria must be established to ensure accessibility, consistency, and reliability. For each of the potential SDLM datasets, the following should be addressed:

- Accessibility & availability: Ideally data used in the SDLM is publicly available at no charge to all stakeholders. For potential data sources, this should be identified.
- Completeness: Data should cover the area of interest. This could be the continental, zonal or member state level. All data should be complete for the study area.
- Up to date: Age of the data is a critical factor. Although some data sources such as soil data are static, others such as weather and cropping data are highly variable. As part to SDLM, guidance should provide on selecting the appropriate dataset, if multiple versions are available, and which dataset should not be considered if the data is considered out-of-date by experts.
- Version control: Is the available data subject to version control and are new versions frequently released? How is this achieved and who is handling this?
- Documentation: Does the dataset have both technical documentation and metadata? A key question here is if the data documentation details the methods used to develop the data, as well as any potential or perceived strengths and weaknesses among other elements.
- Consistency check: The geodata needs to be consistent across the area to be modelled because it does, for example, not make sense to use mixed soil maps of different resolutions and where the properties have not been measured using a harmonised protocol.
- Quality assessment: Data experts should conduct an independent quality assessment of the data to better understand what limitations of the data are and the potential consequences on leaching of pesticides to groundwater.
- Error reporting: A formal procedure to report and correct errors needs to be established.

2.7 Regulatory requirements for the supporting software tools

The regulatory requirements regarding the SDLM software tools should be generally based on the requirements of the Tier-1 FOCUS models. The following points are essential and should be considered if modelling tools should be used within a harmonised framework for SDLM:

- **Compliance with Document on harmonised Approach of SDLM**: The modelling tools should be fully based on the recommendations given in the final document about the harmonised approach. This includes the use of databases, the way the parameterisation is derived from the geodata, spatial and temporal aspects of the modelling as well as target quantities and processing of the data.
- **Version control**: Version control is the central pillar for consistency, transparency and reproducibility of models and scenarios to be used in a regulatory context. Version control ensures that it is transparent for all stakeholders which version of a modelling tool was used in an assessment. It is therefore a pre-requisite for the reproducibility of modelling work. Furthermore, version control helps to standardise and improve the quality of the tools and the modelling work by avoiding that test versions are unintendedly used for assessments. It is also mostly combined with formal and content related quality and plausibility checks of new model versions and hence improves the model quality.The way version control is implemented for the FOCUS Tier-1 models should be the example for the SDLM tools.
- **Open source requirements:** An important aspect regarding transparency is the Open Source of the model codes but also the scenario data that are used in the SDLM tools. This might also

be necessary following the new EU regulation for transparency concerning the registration of pesticides (General Food Law). However, it is necessary to protect the official versions according to the version control (e.g. with a water mark) and prevent that uncontrolled test versions based on modified open source code is used in the registration procedure.

- **Accessibility**: The tools need to be hosted at a central location and should be freely accessible as it is the case for the FOCUS Tier 1 models.
- **Documentation**: A comprehensive documentation is essential especially for reasons of transparency but also to ensure the required user friendliness. It needs to include:
    - The description of the technical basis of the modelling tools. The processes that are implemented should be described or references to documents where this is sufficiently described need to be provided (e.g. to manual of underlying model versions).
    - The description of the geodata that are used for the parameterisation of the scenario including spatial and temporal discretisation and how indirect parameters needed by the models were derived.
    - A manual on how to run the modelling tool.
- **User friendliness**: Options should be provided so that stakeholders (e.g. regulatory authorities) can run SDLM for their own assessments or can reproduce and check existing assessments provided by industry. This includes the user-friendly use of the modelling tools (e.g. via a GUI) but also the possibilities of time efficient solutions and options to run the modelling tools. The option to perform all calculations on a central server with access to all geodata could be investigated. By including the country as an additional map layer, the SDLM-framework could be made operational for national and/or zonal assessments as well.
- **Good modelling practice (GMP)**: For submissions of SDLM assessments within a regulatory framework concerning the registration of pesticides the standards of GMP should be considered. This includes transparent and well justified parameterisation of the modelling tools especially regarding the substance parameters. Aspects of good documentation of the work are also important. They should make it possible to fully understand the assessment and to reproduce it if necessary. Although focussed on ecological models, important aspects of GMP are included in the Scientific Opinion on GMP from EFSA PPR Panel (2014).

3 Spatial and temporal data at the European scale

Models assessing the fate of PPPs in the environment are inherently data intense and become more so, when applied at the landscape level. Irrespective of the model, required datasets can be divided in a limited number of categories including:

1. Soil data (organic matter, particles size distribution, horizons, hydrological properties);
2. Climate and weather data (rainfall, temperature, wind speed, humidity and reference evapotranspiration);
3. Crop and agricultural management data (including irrigation and tillage practices);
4. Groundwater and drainage depth (often optional);
5. Landscape characteristics (in particular slope).

In addition, one or more index grids will be required to a) tie all information together and b) have a unique identifier for each location.

Having well defined and documented datasets are critical towards consistency in the application of SDLM and makes it easier for risk assessors and regulators to understand the meaning of the results.

3.1 Quality criteria

All datasets need to be fit-for-purpose in a regulatory leaching assessment. This means checking the data against the criteria in the EFSA Good Modelling Practice Opinion (EFSA PPR Panel 2014):

1) **Is the dataset well documented?** The following questions could be considered:
    a) Extend and resolution of the dataset;
    b) Description of the underlying data and (pedo)transfer functions;
    c) Ownership of the data;
    d) Release date and procedures to keep the data up-to-date;
    e) Is the dataset subject to Version control by its originators?
    f) License conditions (can the data be used?);
    g) Data format;
    h) Has the data been published and/or used in peer reviewed scientific journals?
    i) Are limitations of the dataset documented?
    j) Does it need to be processed (cleaned) before it can be used?
    k) For what purpose was the dataset developed?
2) Is the procedure for deriving the dataset considered scientifically sound? Particular attention needs to be given to:
    a) The measured data underlying the dataset;
    b) How complete is the data and do we need to develop procedures for filling any potential data gaps?
    c) The statistical upscaling procedures to derive the spatial dataset including (pedo)transfer functions;
    d) Limitations;
    e) The uncertainty of the underlying measurements and (pedo)transfer functions.

3.2 Specific points of attention

Besides the general quality requirements, attention must be given to the following criteria:

- **Spatial and temporal resolution in relation to the scale of the assessment**: Recommendations are needed about the spatial and temporal resolution to be used for SDLM, depending on the spatial scale of the assessment (EU/zonal/national). The focus is at the EU and zonal level; however, recommendations should be given for national assessments as well. Recommendations must include appropriate data resolution (1-km versus 500-m versus 250-

m) that makes it practical to implement and execute such a framework at the intended area-of-interest by stakeholders in the process. The selected resolution may be guided by the exposure assessment goal. For example, a full zonal assessment may likely be conducted at coarse resolution versus an assessment at the sub-member state level. Within one assessment, it is, however, necessary to have a consistent resolution to avoid bias when generating a spatial schematisation.

- **Spatial and temporal resolution in relation to model purpose**: Recommendations must be made about the required spatial and temporal resolution for the respective model purposes (i.e. vulnerability mapping for the selection of groundwater monitoring studies (Tier-4) and spatial modelling (Tier-3b)). A lower spatial resolution may be justified if it is demonstrated that it results in an acceptable approximation of the overall endpoint defined by the exposure-assessment goal. In this respect, the selection of monitoring sites at Tier-4 might need a high spatial resolution, because the monitoring sites refer to given points. Spatial modelling at Tier-3b and setting monitoring data in context, on the contrary, might require less spatial data. If possible, the effect of the spatial resolution on the derived endpoint (80^{th} x 80^{th} percentile) should be tested in order to make recommendations about the minimum requirements regarding the spatial resolution to derive a robust endpoint.
- **Up-to-date**: It is desired to include data that is recent, so that it represents current land cover status and current climatic conditions.
- **Derived data**: There is a distinction between basic data and derived data. Options to derive maps from basic data are pedotransfer functions (e.g. rules for the lower boundary conditions, Van Genuchten parameters for the soil hydraulic functions, rules for the depth distribution of organic matter, etcetera) and geostatistical methods (e.g. procedure to derive grid maps from point observations by kriging). Guidelines should be established what pedotransfer functions are to be used to derive these data.

3.3 Soil data

Currently available datasets

Recommendations are needed on the soil databases to be used. Various soil datasets are currently available, which all have advantages and disadvantages:

- The JRC LUCAS dataset described in http://esdac.jrc.ec.europa.eu/ESDB_Archive/eusoils_docs/other/EUR26102EN.pdf. The JRC LUCAS dataset contains high-resolution maps of organic carbon, texture, bulk density, pH and CEC of the topsoil. For mapping, various (geo)statistical methods have been used, e.g. multivariate additive regression splines (Ballabio et al. 2016). A review of these methods could be done by the geodata working group.
- The ISRIC SoilGrids map described in https://www.isric.org/explore/soilgrids. The ISRIC SoilGrids dataset contains all parameters that are needed by GeoPEARL: organic carbon, texture and *p*H. The advantage of the ISRIC SoilGrids dataset is that it is developed in a transparent manner (R-scripts and data are published in a kind of OpenStreetMap organisation). Moreover, data is generated for multiple depths (3D-soil map). There are, however, considerable issues with the dataset so significant work will be required to make these data work within SDLM.
- The European Soil database: derived data http://eusoils.jrc.ec.europa.eu/content/european-soil-database-derived-data#tabs-0-description=0 . A dataset based on a combination of the World Soil Map and the European soil map is also available. This dataset is based on classical methods of soil mapping using STUs. A gridded version for modelers (derived data) is available.
- The PERSAM dataset http://esdac.jrc.ec.europa.eu/content/european-food-safety-authority-efsa-data-persam-software-tool. The PERSAM dataset has the advantage that all maps have been made available at the same resolution and that they are ready-for-use for EU-wide assessments. There are, however, issues with some of the underlying map layers, e.g. the organic matter map, which is known to overestimate the organic matter content for arable soils (EFSA soil guidance). Also, please note that the resolution of the underlying maps is often coarser than the 1x1 km^2 resolution of the PERSAM maps.

Two main categories
The maps fall into two major categories. The first group of maps consisting of the EU-soil database and the PERSAM dataset are based on the assumption that soil properties within mapped soil polygons are constant. It is well known, however, that soil properties vary within mapped soil polygons. For this reason, a second newer family of soil maps has been developed. These new soil maps have been generated using geostatistical methods for prediction of soil properties in a 3D-space. The JRC Lucas dataset and the ISRIC SoilGrids maps are representatives of this category of maps. Regression kriging is a commonly used technique. This comes down to first building a trend model based on regression with co-variates that are available at high spatial resolution. Then in a second step, the residuals of this trend model are interpolated using geostatistical methods (i.e. kriging). With this second step, local variation of soil properties within (generally large) soil polygons can be simulated.

There are considerable differences between the four datasets. A review of these datasets and recommendations for the final datasets are needed.

3.4 Climate and weather data

Climate and weather data are the second important category of data that needs to be reviewed. The EFSA dataset used the WorldClim database, which is available at a resolution of 1x1 km^2. Like the ISRIC soil data, it is a freely available dataset (https://www.worldclim.org/data/index.html). The WorldClim database appears to be less suitable for precipitation data because the interpolation procedure has some boundary effects. A newer version of the WorldClim dataset is now under development, but it is not clear if this will solve the problems. Another well-known dataset for use at the European level is the MARS database made available by JRC. This dataset is now available at a resolution of 25x25 km^2. Each grid cell is linked to a complete weather series with daily weather data, which means that a realistic spatial pattern of weather conditions is available. This, however, requires a lot of data storage and checking of the data. An alternative is to use multiple grid cells with one weather data file scaled to the conditions of the respective grid cell. The EFSA-dataset, for example, uses one weather datafile for each FOCUS zone. It is furthermore desired that the data is recent, so that it represents current climatic conditions.

So, important tasks of the geodata subgroup is to make recommendations on:

- The database to be used for both the spatial pattern (climatic data) and the temporal pattern (weather data);
- The simulation of potential or reference evapotranspiration;
- The spatial resolution of the weather data to be used (e.g. link one weather datafile to each grid cell or aggregate multiple grid cells);
- The period and length of the time-series.

An important derived dataset is the map of the FOCUS climatic zones. This is an important map layer, because it provides a link to the Tier-1 and Tier-2 assessments, which is based on scenarios for 9 FOCUS climatic zones. Recommendations are needed with respect to this map layer.

3.5 Crop and agricultural management data

Land-use data
The land use/landcover/crop map layer is important, because it is often used as a surrogate of the potential use area of a pesticide. Currently, there is little harmonised crop-data available that covers the entire EU in a harmonised way. To the best of our knowledge, the CAPRI dataset extended with information on permanent crops is the only such dataset currently available. This dataset is made available in the EFSA spatial dataset (EFSA 2017). However, the CAPRI-data is more than 10 years old and a dataset describing more recent conditions is desired in the SDLM-framework. Recommendations on an update should be part of the remit of the geodata working group.

Crop characteristics

Crop development stages and properties such as the LAI, crop height and crop factor are available in the FOCUSgw dataset (FOCUS 2009; EC 2014) and are also used in the EFSA spatial dataset (EFSA 2017). The advantage is that the parameters in this database have common agreement in the regulatory area. The disadvantage is that the data is only available for the nine FOCUSgw zones, which makes a more targeted assessment uncertain. The alternative would be to use a crop simulation model like WOFOST for crop development, but this would require a lot of effort. A mixed approach is possible as well. In this approach, the emergence and harvest dates are modelled based on the temperature sum, whereas the other parameters are continued to be used. This approach is used in e.g. the FROGS model (Beigel et al. 2014 and in Tiktak (2012). When making recommendations for the crop factor, attention must be paid on how the potential evapotranspiration is modelled and/or input into the model.

The crops in the crop map layer (e.g. the CAPRI dataset) might differ from the crops in the FOCUS dataset. Clear guidance on how to link both datasets is needed (see e.g. Table 6 in EFSA 2017).

Interception and wash-off

Crop interception may be included in the SDLM-framework. Since the introduction of the FOCUS groundwater scenarios, it has been common practice to reduce the application rate by the fraction that is intercepted by the crop canopy and to apply this reduced fraction to the soil (EC 2014). As described by EFSA PPR Panel (2010), this approach is not considered defensible because there is insufficient evidence that wash-off from the crop canopy can be ignored. The effect of dissipation at the crop canopy and foliar wash-off should be included as an option in the SDLM-framework. This provides the option to include these processes as soon as Tier-1 and Tier-2 are updated. Recommendations are therefore needed on how to incorporate these processes in the SDLM-framework.

Agricultural management including irrigation

Irrigation has a huge impact on the leaching of pesticides. Recommendations are needed on how to simulate irrigation, and in which crops and climatic zones irrigation is applied. The procedure used in EFSA (2017) could serve as an example. Recommendations are further needed on tillage practices. Eurostat statistics maybe helpful to improve agricultural management schemes.

Crop rotation

An important assumption of the current FOCUS models is that there is no crop rotation, so the same crop is used each year. It is technically possible to include crop rotation (see e.g. Beigel et al. 2014 for France); however, Ziółkowska & Topping (2019) demonstrated that it requires a lot of effort to obtain these data. Furthermore, there are hurdles with respect to privacy of census data, which are needed to obtain sound crop rotation schemes for various farm types. Crop rotation will therefore not be included in the SDLM-framework for the time being. The currently used FOCUS approach (application each year, biennially or triennially) will be used as a surrogate instead. If future developments would make data on crop rotations more easily available, future working groups could investigate the option to include crop rotation in a more realistic way.

3.6 Groundwater and drainage

Lower boundary condition of the hydrological model

For accurate simulation of the mass flux going into groundwater, it must be known which part of water and pesticides applied drains to the surface water and/or is lost by surface runoff (and interflow). As far as we know, there are no maps of this interaction available at the European level. So, we need to work with pedotransfer functions and/or rules. The idea behind this is, that soil profile information gives a good indication of these interactions. Centofanti et al. (2008) described the lower boundary condition of the MACRO model as a function of substrate material, depth to a slowly permeable or impermeable soil layer and soil water regime as used in the Hydrology of Soil Types (HOST) system (Schneider et al. 2007). This method has successfully been applied in the EU-funded FOOTPRINT project (Centofanti et al. 2008), but has never been readily available to the modelling community as a whole. The geodata subgroup could elaborate on the possibility to make this procedure work within the SDLM-framework.

Groundwater depth

Recommendations are needed on datasets to obtain depth to the groundwater, e.g. to restrict the assessment to shallow groundwater sites (e.g. Fan et al., 2013). Seasonal variability of groundwater tables could be included in the assessment. Recommendations are further needed on the occurrence of karstic soils depending on the soil depth the karstic structures can be found. Although the endpoint for the SDLM-modelling is 1-m depth (Chapter 2), recommendations on soil profile descriptions below 1-m depth are welcome. The latter could help harmonising the interpretation of groundwater monitoring studies at Tier-4.

3.7 Landscape data

If overland flow is to be included, landscape properties become important. Although slope is not a factor in generating overland flow, it is important in determining the storage capacity at the soil surface. An EU-wide slope map derived from a Digital Elevation Map is available at the Eurostat website https://ec.europa.eu/eurostat/web/gisco/geodata/reference-data/elevation/eu-dem/slope.

3.8 Recommendations for version control and maintenance

This section should give recommendations on how the database for the SDLM-modelling should be maintained. In principle, the responsibility for maintaining the original dataset remains at the data owners. There is, however, a potential problem here, particularly if the data is created only once as is the case with the OCTOP map and with the CAPRI dataset. And secondly, recommendations are needed on how to deal with updated datasets if flaws are found. So, recommendations should include:

- Maintenance of the original and derived dataset(s);
- Options for a common data platform, e.g. the JRC-website;
- Version control (inside or outside FOCUS version control?);
- A process for correcting error.

3.9 Remits for the geodata subgroup

Objectives

The objectives of the geodata subgroup are:

- To define the data requirements for SDLM;
- To make an inventory of all data sources needed for SDLM;
- To make an assessment of the content (temporal, spatial) of the data sources;
- To assess the quality of the data sources and review options to improve the quality where needed or fill data gaps;
- To review options for common data platforms, maintenance and version control;
- Recommend which data sets to use for the various aims of the SDLM;
- Recommend how to process said data sets;
- Recommend for temporal data an appropriate time period that data should cover;
- Document pitfalls for datasets and or lists data sets not to use
- Recommend and develop a procedure for correcting errors.

Procedure

Several members of the SETAC SDLM steering committee will join the geodata subgroup. Additional experts outside the SC will be nominated following recommendations by members of the SC. The chair and co-chair of the subgroup will be nominated by the steering committee. The subgroup will organise at least two meetings a year to discuss the subgroup activities and to temporally invite additional external experts when needed. The subgroup has to prepare a report by the end of the second year after the subgroup has started.

Expected results

The deliverable of the group is a report or a section of a single overall report of the working group, in which the data needed and their use is described for SDLM for regulatory use within the EU.

Time schedule
The subgroup is to be formed during the first meeting of the SETAC SDLM working group. The lifetime of this subgroup is two years, but this may be longer if needed.

4 The modelling framework

The working group needs to make recommendations of the models and tools that are seen appropriate to be used for SDLM. The focus should be on models which are already used for (lower tier) leaching assessments in the current EU registration procedure and for which also experience exists with spatially based approaches (e.g. it should be feasible to run the model for a continental/sub-continental level). For this initial phase of the SDLM project, modelling will be focused on the vertical downward transport through the (mostly) unsaturated soil zone (like FOCUS Tier-1). Sophisticated model combinations to account for groundwater hydrology are not foreseen in this phase. This does of course not exclude simple approaches to somehow account for lateral groundwater flow, e.g. when the groundwater is shallow, and drainage is likely to be an important loss pathway. Recommendations could also include the potential use of alternative methods such as index methods and metamodels (e.g. as presented in FOCUS, 2009) which may significantly reduce computation resources.

4.1 Two different goals

The modelling frameworks should serve two different goals:

- **Tier-3b** requires the simulation of a frequency distribution of the leaching concentration, which should be in line with the FOCUS exposure assessment goal (i.e. the 80th-spatial percentile and temporal percentile at 1-m depth). The user should be able to also introduce parameters of process refinements in accordance with Tier 2a (Figure 1) of the FOCUS tiered approach (e.g. aged sorption, pH-dependent sorption etc). So, there is a need for a rather sophisticated leaching model (e.g. PEARL, PELMO or MACRO). The drawback of such a sophisticated model is the computation time. So, the characteristics of Tier-3b simulations are a high level of process sophistication at the cost of a lower spatial resolution. It is, however, well known that a higher spatial resolution generally leads to more extremes and hence a higher P80-value (see e.g. Heuvelink et al. 2010; van den Berg et al. 2012). Sensitivity analysis should reveal which resolution gives an acceptable compromise between the specific exposure assessment goal and practical considerations such as the computation time (see section 4.3).
- SDLM at **Tier-4** can be used for in context setting of monitoring sites and for site selection (see Chapter 2). The same model (e.g. GeoPEARL) can be used for Tier-3b and for Tier-4. However, at Tier-4 the purpose is only to rank sites or locations and not to model a leaching concentration. Therefore, other methods such as index method or the use of metamodels as described in FOCUS (2014) could be helpful as well.

4.2 Tier-3b leaching assessment

Tier-3b aims at almost the same exposure assessment goal as Tier-1 and Tier-2, so it will deliver the 80th-spatial percentile of the 80th-temporal percentile leaching concentration in the area of use at 1-m depth. The model must be able to handle all parameter refinement options introduced in Tier-2, e.g. aged sorption or *p*H-dependent sorption. If possible, the user must be able to use the same substance database to avoid duplication of work. Added values of Tier-3b above Tier-1 and Tier-2 are: (i) the model can be used for certain use areas, (ii) the model can be used for correctly modelling the exposure assessment goal for substances whose environmental fate properties depend on soil properties other than organic matter (e.g. clay content or pH), and (iii) mitigation options by excluding vulnerable areas or drinking water extraction areas can be investigated as well.

4.2.1 Schematisation procedures available

To reduce the runtime, a schematisation is needed at Tier-3b using a statistically sound clustering procedure. The quality of the schematisation should be such that the frequency distribution of the schematisation equals the frequency distribution of the full model as well as possible. This should be checked by sensitivity analysis, e.g. running the model for each pixel in the use area and see how well the scenarios reproduce the frequency distribution. There are several options available for schematisation, that need to be discussed by the WG:

- The first method consists of **simply selecting pixels** from the full map. This results in e.g. 1000 model scenarios. To get the best schematisation, selection could be done using a stratified random sampling procedure. The advantage of this procedure is that it is relatively simple to perform, the disadvantage is that it just results in a number of scenarios and not in a full map of the leaching concentration. The last point could be resolved by applying statistical interpolation (kriging) on the final results, but this requires more effort from the user.
- The second method is based on **clustering the original map layers**. This is the procedure that is used in GeoPEARL, EuroPEARL and the FOOTPRINT-project. There are several techniques available for clustering. A promising method for which user-friendly software has been developed (Van den Berg et al. 2017) is called *k*-means clustering. This procedure was also used in the FOOTPRINT-project (Blenkinsop et al. 2008; Wiks 2005). This procedure works best with continuous map layers (e.g. organic matter), but its use is limited when many categorical map layers such as land-use are included. This procedure is slightly more complicated than the first procedure, but the advantage is that both a map and a frequency distribution are generated.

  Within the clustering procedure, there are again two main choices to be made, for which the WG needs to make recommendations:
  a) Within each cluster, **a single scenario** is selected to represent the entire cluster. E.g. the scenario that is closest to the mean organic matter content of the entire cluster.
  b) **The average of all pixels** within a cluster is used (this is the procedure currently used in GeoPEARL). This method is easier to apply than the earlier method, but the drawback is that averaging will generally result in lower leaching concentrations (Heuvelink et al. 2010).

Map layers to be included into the schematisation could be:

- The generalised land-use map as derived from the CORINE land-cover database. The following categories are distinguished: annual crops, grass, permanent crops, rice and non-agricultural (the last two categories are not relevant for the Central Zone);
- The soil textural map of Europe. The following categories are distinguished: Coarse, Medium, Medium Fine, Fine, Very Fine and Organic;
- The map with FOCUS zones. The following zones are distinguished: Jokioinen, Châteaudun, Hamburg, Kremsmünster, Okehampton, Piacenza, Porto, Sevilla and Thiva. This map is needed, because many model parameters are derived for FOCUS scenarios;
- Organic matter content of the top 30 cm of soil based on the OCTOP map (if data is available on organic matter content between 30 and 100 cm, this would be welcome as well, because this affects also the leaching vulnerability);
- Mean annual temperature as derived from the WorldClim or JRC MARS database;
- Mean annual precipitation as derived from the WorldClim or JRC MARS database;
- The map of EU-countries. The advantage of including this map in the spatial overlay is that target variables could also be derived for individual countries;
- Maps of categories showing the interaction with the groundwater system based on e.g. the HOST-system.

4.2.2 Considerations for the WG

Developing the best procedure for schematisation needs to be part of the remit of the WG. There are some considerations:

- **The quality of the schematisation** must be checked by sensitivity analysis. It is particularly important that the P80-value is well represented by the schematised model. In such it is important to realise that adding more scenarios might lead to a higher P80-value.
- There is no unique schematisation for each substance and for each crop type. This means that it must be possible **to generate a schematisation "on the fly"** by an automated and well reproducible procedure.

- It could be an option **to start with a limited number of scenarios** and only do more work if needed (this option is available in the Dutch version of GeoPEARL).
- It must be possible to select part of the area, e.g. to model the effect of mitigation measures (e.g. exclude karstic areas).

4.3 Tier-4: site selection and setting monitoring sites in a wider context

At Tier-4 SDLM can be used for two purposes, putting monitoring sites into context and selection of candidate locations and/or regions in which to site monitoring wells. The same model (e.g. GeoPEARL) can be used for Tier-3b and for Tier-4. However, because the purpose of SDLM at Tier-4 is only to rank locations and not to simulate a concentration, alternatives such as the index method or the use of metamodels as described in FOCUS (2014) could be helpful as well.

This section discusses the use of SDLM for site selection and for context setting. It also briefly discusses some additional considerations for the selection and interpretation of groundwater monitoring studies. This includes such items as travel times and connectivity between the field (1-m depth) and the actual monitoring well. It does not, however, discuss site instrumentation, product use history, hydrology surveys, monitoring study conduct including analytical methods; this is discussed in Gimsing et al. (2019).

4.3.1 Use of SDLM for site-selection

At present there is no generally available soil dataset that can be used to identify potential monitoring sites at a field-level across the EU. It is unlikely that one of sufficient quality will become available during the operational lifetime of the group and the computational burden involved in performing SDLM on every field in Europe is at present too large to make this a practical option. Nevertheless, SDLM is a helpful tool to select regions in which to site groundwater monitoring wells in the pre-selection phase. For example, knowledge of whether regions in northern or southern Europe are likely to be more vulnerable for a particular molecule and use-pattern can be useful when designing a monitoring study to target sites in appropriately. A particular advantage of SDLM for this purpose is that it provides a clear and reproducible rationale for site selection at the regional level. However, it needs to be understood that results from SDLM are only a starting point of site selection. Hence, site selection consists of two phases:

- Selection of vulnerable areas and/or regions (preselection phase);
- Selection of the actual monitoring sites within these vulnerable areas.

Preselection phase

SDLM plays an important role in the **preselection phase** because it provides probably the only way of estimating vulnerability of groundwater to leaching of a chemical in a consistent way across all the EU and of comparing leaching vulnerability of one location compared to another. There are some questions to be addressed by the working group:

- Which metric is most appropriate to use for vulnerability assessment from those available (e.g. concentration, mass flux etcetera)? If a different metric is chosen than the metric used for the exposure assessment goal at Tier-1, Tier-2 and Tier-3b, differences need to be analysed by the working group.
- At which spatial and temporal scale should the vulnerability assessment be done? SDLM at Tier-3b is likely done using a spatial schematisation using unique combinations of soil type, weather conditions, etcetera. Is this resolution sufficient for selection of vulnerable areas and/or regions?
- Are there any substances for which the use of currently used versions of SDLM would be inappropriate? For example, substances that do not show significant correlation between leaching and soil properties included in currently available leaching models or substance that show an extreme variability of substance properties? If the SDLM would be invalidated for specific substances, would there be other feasible means of comparing leaching vulnerability at an EU, FOCUS Zone, Zonal or National level?

- Given that the vulnerability assessment at Tier-4 is aimed at ranking locations, would simpler alternatives such as index methods and/or metamodels be applicable as well?

Selection of monitoring sites
Once a region has been selected using the SDLM, monitoring sites within that region need to be selected. This final selection is outside the scope of the working group because consideration of product use history, groundwater depth and travel times are not directly relevant to SDLM; the work of the Working Group will concentrate upon the preselection phase. Nevertheless, some practical aspects of the final site selection are relevant to the preselection phase:

- In practice monitoring studies are likely to encounter a high rate of drop-out of potential sites, due to a combination of unsuitable site characteristics, unwillingness of site owners to participate in a study and lack of product use, amongst other factors. The group will need to make recommendations on the validity of considering regions in a broad percentile range, rather than a narrow one (i.e. such as 90 – 95% vulnerability) to accommodate this rate.
- The group should provide recommendations on the potential for the GIS to represent actual conditions at field locations i.e. soil characteristics, weather and hydrology are unlikely to be the same as indicated by the GIS.

For consideration of the final site selection process, the reader is directed toward Gimsing et al (2019) where these topics are addressed directly.

4.3.2 Use of SDLM for in context setting of monitoring sites
Once a monitoring site has been selected and wells installed, site characteristics can be used as input into models and compared with the output of SDLM. This process is called context setting. Context setting of monitoring sites therefore, comes down to comparing the leaching vulnerability of the monitoring sites with the frequency distribution obtained from the SDLM-simulations (see Gimsing et al. 2019 for examples).

SDLM as proposed here might not be the appropriate tool in all cases. Recommendations are therefore needed on how to interpret results from the in context setting and actions that can be made on this basis. Some key considerations for context setting are:

- How should the context setting of sites be interpreted? The actual groundwater vulnerability presented by a site will likely be due to a combination of factors not represented in the SDLM such as groundwater depth, aquifer characteristics and crop rotations. Does context setting provide a valid estimation of the vulnerability of a particular site?
- Does the output of SDLM sufficiently represent the overall vulnerability of the monitoring sites? The proposed SDLM-version is limited to the top 1-m. Depending on substance properties, it can take decades for a compound to reach typical well screen depths that sample the upper groundwater of an aquifer. How can vulnerable wells be excluded that would produce only false negatives if not extended sufficiently long enough? How can the recommendations given in Gimsing et al., 2019 regarding the substance travel time (time of flight) be included?
- What are the appropriate metrics for comparison, e.g. flux weighted concentration, resident concentration or mass flux?
- Is the area of use sufficiently covered by the SDLM (is the shape of the frequency distribution sufficiently well described by the SDLM-modelling)?
- Does context setting allow for results from one monitoring site to be extrapolated to another at a Member State, regional or Zonal level?
- Which soil data should be used for context setting of monitoring sites once these have been selected and wells installed? Should local data (e.g. from measured soil profile data from the borehole of a well) be used for the quantitative leaching assessment of the neighbouring field as a basis for comparison with the SDLM cumulative distribution function (CDF) curve? Or should GIS data that describes the monitoring site be used?

4.3.3 Additional considerations for the interpretation of public monitoring studies

Monitoring data at Tier-4 can consist of two different types of study (Gimsing et al. 2019):

- A dedicated monitoring well network designed by notifiers to demonstrate the safety of the product;
- An existing public monitoring network not specifically designed for demonstrating the safety of a single product.

In dedicated monitoring studies, often, monitoring wells are situated at edge-of-field. The relationship between the exposing field and monitoring well are therefore known and parameterisation of the SDLM with field data may be valid. With an existing monitoring well network this relationship may not be so clear. For example, the use of public monitoring data can involve the use of monitoring wells at a greater distance than edge-of-field and it may not be possible to know whether a single or multiple fields are connected to the well. The applicability of SDLM in context setting these different types of situation needs to be considered.

4.4 Model Selection

Compatibility with Tier-1 and Tier-2

As mentioned in Section 4.1, the model selected must be able to simulate processes that are included in Tier-1 and Tier-2. This means that the model descriptions and parameterisations in EC (2014) serve as a benchmark. Because further harmonisation of e.g. aboveground processes and crop development has been performed during the development of the EFSA soil guidance, it is also essential that EFSA (2017) is taken into account. FOCUS_PEARL and FOCUS_PELMO have already gone through this process. If other models (e.g. MACRO and PRZM-GW) are added, it is essential that they are benchmarked against these two models and that process descriptions and parameterisations are harmonised where possible.

Lateral flow processes

As described earlier, the FOCUS models are 1D-models, so lateral flow and loss processes are ignored. Consensus therefore need to be reached in the WG to describe these lateral flow processes, in particular surface runoff and drainage. Because drainage occurs in the saturated soil, description of the interaction with the groundwater is an essential component.

Practical considerations

The models must follow the requirements of the EFSA GMP opinion. In addition, the following points need to be addressed:

- **Process descriptions:** Processes included at the lower tier also with regard to parameter refinement such as pH-dependent or aged sorption must be included, either explicitly or implicitly when using a metamodel approach. Regarding the process of preferential flow, it was already discussed in Chapter 2 that although it would make the assessment more realistic, no harmonised method is available to derive the parameters needed for describing preferential flow at the regional scale. Furthermore, this would have consequences for the tiered approach because the inclusion of preferential flow at the higher tier would probably invalidate part of the FOCUS scenarios because it could lead to higher leaching concentrations. It was therefore decided that it is out of scope of the working group to develop a preferential flow version. If an agreed methodology becomes available for Tier-1 and Tier-2, this can be introduced in the SDLM framework after revision of Tier-1 and Tier-2.
- **Validation status**: The system needs to be tested and compared to calculations with single Unique Combinations using the respective FOCUS model. Plausibility checks also need to be performed.
- **Documentation**: The system needs a document in which the data used, the model concepts, the model output as well as the way the system can be run is described in a comprehensive and transparent way.
- **Version control**: Version control similar to that for the FOCUS software packages is necessary.

- **Accessibility:** The modelling tool needs to be accessible to all relevant stakeholders. There needs also to be a possibility for risk assessors to access the system to test or reproduce results that are submitted.
- **Maintenance**: Needs to be ensured for more than 5 (better 10) years.
- **Performance**: The system must be accessible to regulators. Runtime should preferably be less than 24-hours on the platform offered. The tool must have a user-friendly interface.

4.5 Remit of the modelling subgroup

Objectives
The objectives of the model framework subgroup are:

- To define the model framework requirements (spatial and temporal) for SDLM at both Tier-3b and Tier-4;
- To define and evaluate the modelling tools needed within the SDLM framework;
- To develop a method to handle all parameter refinement options introduced in Tier-2, e.g. *p*H-dependent and aged sorption in the model framework;
- To review the additional processes that need to be included in the model components of the framework. This should include a review of lateral flow processes, the interaction with the groundwater and the handling of crop rotation. A review of the possibility for including preferential flow is welcomed; however, given the limited time available, it will not be possible to include this process yet (Chapter 2). The consequences for adding additional processes for the tiered approach must be assessed as well;
- To assess the spatial maps generated by the geodata subgroup needed to prepare an appropriate schematisation for use at Tier-3b;
- To give recommendations on the use of derived data such as pedotransfer functions;
- To develop a methodology to derive a schematisation for the model framework;
- To develop a first version of the model framework;
- To prepare a series of tests to demonstrate the use of the modelling framework;
- To review options for common platforms, maintenance and version control;
- To perform a plausibility check of the Tier-4 vulnerability approach using existing datasets.

Procedure
Several members of the SETAC SDLM steering committee will join the modelling subgroup. Additional members will be nominated by the members of the SC. The chair and co-chair of the subgroup will be nominated by the steering committee. The subgroup will organise at least two meetings a year to discuss the subgroup activities and to invite external experts when needed. The subgroup has to prepare a report by the end of the second year after the subgroup has started.

Expected results
The deliverable of the subgroup is a report or a section of a single overall report of the working group. This report should include a description of

- the modelling framework including its components and schematisation;
- new processes, particularly considering the interaction with the groundwater and lateral flow processes;
- its use for regulatory purposes (i.e. Tier-3b and Tier-4 assessments).

In addition, the subgroup will deliver a set of operational model framework components to demonstrate its intended use for regulatory purposes within the EU.

Time schedule
The subgroup is to be formed during the first meeting of the SETAC SDLM working group. The lifetime of this subgroup is two years, but this may be longer if needed.

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