Workshop
on
Spatially Distributed Leaching Modelling of Pesticides

24 May 2019
Ghent, Belgium

Initiated by
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Abstract

This report summarises the outcomes of a Workshop on Distributed modelling convened by a panel of experts at the IUPAC international conference in Ghent Belgium in May 2019. The workshop consisted of international experts in GIS and groundwater modelling and was comprised of representatives from academia, regulatory authorities, research institutes, contract organisations and industry. The workshop was convened in response to resolutions passed at the 9th European Modelling workshop in 2018 in Copenhagen.

Distributed modelling is the term used to describe the pairing of models and GIS data to provide estimates of potential environmental concentrations at a landscape level. Some Member States (such as the Netherlands) use this approach as a higher Tier option in their national groundwater exposure assessments, and provision for this approach also appears in FOCUS groundwater at Tier 3. However, there is at present no guidance for how to perform such modelling studies at the EU level with the available models and GIS data. This type of modelling has also been used to identify vulnerable sites to monitor groundwater and could potentially be used to place groundwater monitoring sites in context of a European distribution as outlined in the report of the SETAC EMAG-Pest GW working group (Gimsing, A.L., Agert, J., Baran, N. et al. J Consum Prot Food Saf (2019) 14(Suppl 1): Conducting groundwater monitoring studies in Europe for pesticide active substances and their metabolites in the context of Regulation (EC) 1107/2009).

The need to provide guidance to regulatory authorities and the wider scientific community on how to perform and interpret distributed modelling studies at the European level was recognised at the 9th European Modelling workshop and provided the motivation for this meeting. It was also recognised that the available GIS data itself needed to be considered in addition to how it was used to parameterise models. In particular how these data can be quality checked and used in a version control process similar to that used for modelling.

Results and resolutions passed at the workshop are presented in the areas of GIS modelling, GIS data and for regulatory aspects. The report also presents options for developing guidance in the area of distributed modelling of groundwater and addresses version control.
Motivation for This Workshop

In general, there were two main reasons that motivated the organizers of this workshop to start the initiative on a harmonized framework on spatially distributed leaching modelling (SDLM):

1. In the resolutions of the 9th European Modelling Workshop in 2018 in Copenhagen the following was concluded:
   a) A dialog is needed on a spatial modelling framework needed for:
      - selecting appropriate monitoring sites
      - setting existing sites into context
      - requirements on input and output of appropriate spatially-distributed models
   b) Version control is needed for high-resolution spatial databases for the EU

2. Spatially distributed modelling is already used for higher tier modelling leaching assessment by some member states (e.g. GeoPEARL in NL). Since it is also included in FOCUSgw higher tier as Tier 3 it will probably become more important in future on EU and MS level. This requires guidance and harmonization to increase the quality and acceptance of this approach.

**FOCUS gw higher tier 2009 (2014)**

![Diagram of tiered approach](image)

Figure 1: Scheme of tiered approach taken from FOCUSgw higher tier report (FOCUS, 2014). Areas where SDLM is needed or can be used are highlighted.
Basic Requirements for Spatially Distributed Leaching Modelling Systems

The organizers of the workshop agreed that the modelling systems need to meet at least five basic requirements to achieve a sufficient level of acceptance by stakeholders comparable to the Tier 1 FOCUS leaching models.

1) **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.

2) **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.

3) **Version control**: Version control similar to that for the FOCUS software packages is necessary.

4) **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.

5) **Maintenance**: Needs to be assured for more than 5 years.
WORKSHOP ON SPATIALLY DISTRIBUTED LEACHING MODELLING

Ghent, Belgium

24 May 2019

Final program

8.30 – 9.00 Coffee/tea

First session: Workshop target and key-note speakers

9.00 – 9.15 Welcome by organizers and workshop target

9.15 – 9.30 Introduction of participants

9.30 – 9.50 Keynote lecture Aaldrik Tiktak (PBL, The Netherlands)
Elements and options for a spatially distributed modelling framework

9.50 – 10.10 Keynote lecture Anton Poot (Ctgb, The Netherlands)
Experiences using spatially distributed models in the Netherlands – a regulatory perspective

10.10 – 10.30 Keynote lecture Michael Stemmer (AGES, Austria)
Experiences using spatially distributed models in Austria

10.30 – 10.45 Coffee break

10.45 – 11.05 Keynote lecture Paul Sweeney (Syngenta)
Experiences using spatially distributed models – an industry perspective

11.05 – 11.25 Keynote lecture Marc van Liedekerke (JRC, Italy)
Characteristics, availability and quality control of geo-spatial data for spatially distributed modelling

11.25 – 12.25 First session breakout discussion groups
topics discussion groups: 1 input data, 2 model requirements, 3 regulatory aspects
12.25 – 12.45  First plenary session: summary of breakout sessions
Chairs: Erik van den Berg and Gerco Hoogeweg

12.45 – 13.15  Lunch

13.15 – 14.00  Second session breakout discussion groups
topics discussion groups: 1 input data, 2 model requirements, 3 regulatory aspects

14.00 – 15.00  Second plenary session: results breakout discussion groups, recommendations and follow-up actions
Chairs: Bernhard Jene and Erik van den Berg

15.00  Closure of workshop
Envisioned Outcomes and Next Steps

The organizers agreed on the following basic points that are envisaged as results of the SDLM workshop:

- Agreement on need for framework for SLDM supported by MS
- Inventory of model concepts and data requirements
- Preparation of workshop report with summary of discussions on subtopics data, modelling framework and regulatory aspects as well as recommendations
- Identify a member state that could lead this effort
- Alignment with SETAC EMAG-GW

As next steps the following two points were envisaged by the workshop organizers:

- Joint meeting with SETAC EMAG-Pest GW working group (Piacenza Sept 2, 2019) to discuss on how to proceed with this initiative
- Presentation of the summary of findings at the Pesticide Chemistry Symposium in Piacenza 2019
Results of Breakout Sessions

Conclusions from Breakout Group 1 On Input Data
Moderators: Paul Sweeney and Gerco Hoogeweg

This group addressed a wide variety of data related topics ranging from which data should be used to represent soil, cropping and weather to how to ensure that GIS data are of enough quality and the process for hosting and quality-checking data. Soil data for the EU is a key area of uncertainty as there are different data available (e.g. SPADBE and LUCAS) and no general acknowledgement which of these data best represent soils in European agricultural areas. They also are of different qualities and resolutions.

Often the purpose of the dataset is not stated in the documentation, so it is difficult to define appropriate use. Similarly, there was no generally acknowledged body to consult on which of the available datasets should be used. The group proposed that a user group is to be established to recommend appropriate use of data in support of distributed leaching modelling. This may help to gain a greater level of trust among Member States. At present the acceptance of EU data differ between Member States.

The group made recommendations for use of datasets where there were limited options. The larger SDLM group was requested to provide feedback for why that choice of data layer might be inappropriate at the EU and zonal level. The following datasets for pan-European and zonal modelling frameworks were recommended:

- **Weather:** MARS25km
  - Questions remain which period should be modelled
- **Crops (Spatial filter i.e. to define agriculture/non-agriculture)**
  - CORINE permanent crops
  - NUTS 3+ level data
- **FOCUS Zones**
  - Should be defined from the weather data used in the modelling.

The following issues were identified with other data layers

- **Cropping**
  - Can we use EU Statistics database to determine by FOCUS zone and member states if to apply irrigation?
- **Groundwater**
  - What does shallow groundwater mean?
  - How to handle fluctuating groundwater table?
- **Soils (two options were available)**
  - ESB (Derived), EFSA OM, SOILGRIDS (ISRIC)
  - New soil layer development what if we amend LUCAS data (if done to protocol)

The group also debated the following topics and made the following observations:

**Data Limitations**

- Unrealistic values are often present in dataset and how should modellers treat these values?
  - pH map is an example
- How to improve databases (existing ones)?
• EU versus National Level versus Field (different requirements?)
• ESDB not suitable for vulnerability mapping?
  o Potential introduction of bias?
• How can we facilitate data for distributed modelling?
  o JRC needs a project from which the data can be generated
    ▪ Right people official nominees
  o Evaluate databases for SDLM?

Data Acceptance
• ESDB is not accepted by some MS
• For some areas no organic matter data available

How to Define a Protection Goal?
• See regulatory session. This topic should be addressed there.
• Hard to define and very diverse
• Feedback from authorities are virtually not existent

Weather Data
• WorldClim
  o Monthly data only, thus not useful in most spatially distributed modelling efforts with daily-time step models.
• What alternatives to MARS25km exist and are consistent across the EU?
• MARS 25km is the most useful dataset
  o Time series with daily data
  o Generally accepted by most MS if not all
• What time period to use?
  o At least 6 warming-up years are required and 20 years for evaluation.
  o For tri-annual application we need 60 years of data (repeat of the 20 years?)
• What to do with extremes and errors?
• How to derive the FOCUS zones?

Land Use and Cropping Data
• CARPI does a good job, but some crop classes are poorly documented and there are known data gaps
  o Data is from before 2000
• Is being updated
• ESA satellite data and alternative source?

EFSA Data
• Collaboration agreement still exists

JRC
• The organization is official, but the data is not official
  o Perception is that JRC’s data is the “official” data from the EU
  o Who can certify this information?
  o Can you improve data and acceptance at the MS level?
• ESDB is used are co-variate in e.g. LUCAS
• At present (May 2019) no new data foreseen just yet coming from JRC
• E.g. Soil database X to be for SDLM, expert review and rec changes
• SinFo (by MARS for crop forecasting)
• JRC is a liaison with EU Soils Export Group
• How does SOILGRIDS fit in?
• Not all JRC data are quality checked
Conclusions from Breakout Group 2 On Modelling Requirements
Moderators: Erik van den Berg and Michael Klein

General

Over the years the performance and capacity of computers have increased enormously. Further, new methodologies have been developed to distribute computational tasks, e.g. by using cloud-based services. Therefore, computational time and processing large amounts of data have become less problematic or difficult.

The requirements for a model framework for putting monitoring sites into context are different from those for a framework to assess the leaching concentrations at the evaluation depth, currently 1 m in the EU.

For a model framework a link with a groundwater model is necessary but for the assessment of the leaching risk it is not.

Assessment of leaching to groundwater

All relevant processes need to be included. In the current FOCUS leaching scenarios macro pore flow is not considered, whereas the occurrence of macro-porous soils within the EU is widespread. Further, both run-off and drainage are processes that need to be considered in the schematisation for the leaching assessment

Important elements to be addressed

- testing the models at field-scale against measurements from field experiments
- regional differences in water recharge drainage should be considered when preparing the model input data
- regional data on the partitioning of the water flow in the soil to groundwater or surface water could be helpful in the schematisation of the region for the modelling framework
- stagnant groundwater may occur in specific areas

Interpretation of monitoring data

Linking a leaching model with a groundwater flow model is essential. As a first step, a simple approach can be adopted, e.g. by assuming a single groundwater layer with specific thickness and water flow rate. This approach is applied by VITO. Given the variation in monitoring data the model framework and its components need to be flexible.

Important elements to be addressed:

- bottom boundary condition. Possibly free drainage could be assumed as a first step
- depth dependent transformation needs to be considered
- method of coupling 1-D leaching model to groundwater flow model
- procedures developed for the Water Framework Directive may be helpful
Conclusions from Breakout Group 3 On Regulatory Aspects
Moderators: Bernhard Jene and Robin Sur

First discussion round
The following points were used to stimulate the discussion about the use of SDLM in regulatory context for the first breakout group on regulatory topics:

- Possible benefits of SDLM in regulatory context (EU level, MS level):
- SDLM in context of other initiatives (e.g. SETAC EMAG-Pest GW, MAgPIE)
- SDLM and localized / regionalized risk management
- Pre-condition for regulatory acceptance of SDLM

Near future benefits were predominantly seen in supporting monitoring studies by performing vulnerability analysis to either selecting monitoring sites that cover sufficient vulnerability or to set monitoring data from existing sites into context.

The discussion was mainly focused on the specific protection goal in groundwater (SPGgw). The majority was of the opinion that a SPGgw would be necessary for the evaluation of results from SDLM before it could be used as higher modelling tier for the EU leaching assessment (Tier-3b). It was argued that implicitly a SPGgw is used for the Tier 1 FOCUS scenarios (90\textsuperscript{th} percentile in space and time of the simulated annual soil pore water concentration at 1 m depth on field level, e.g. 1ha). Theoretically this could be easily transferred to the higher tiers of the groundwater assessment scheme such as SDLM and monitoring. But it was mentioned that this SPGgw would need a revision since it was defined 20 years ago. On the other hand, it was discussed that SPGs should be consistent across all four tiers which would make it easier to agree on a common SPG on Tier-4.

Communication problems regarding the SPGgw were identified. The Water Framework Directive refers to groundwater that can potentially be used for drinking water. Therefore, it needs to be determined which percentile in groundwater does fit to the overall 90\textsuperscript{th} percentile target?

The general opinion was that the definition of a SPGgw would be less important if SDLM should be used to support the selection of vulnerable sites for groundwater monitoring or to determine the vulnerability of sites that were used in a groundwater monitoring study. A certain percentile for the vulnerability of a site, e.g. based on simulated substance loads over a representative time period (e.g. one year), can be calculated to support the selection of monitoring sites in a targeted groundwater monitoring study. It was concluded that a lot of work was already done and presented in the SETAC EMAG-Pest GW report. Nevertheless, discussion about the appropriate quantity to judge on the vulnerability is essential. It needs to be decided whether leachate or pore water concentrations or leached substance mass should be used and if absolute or relative values (e.g. percentage of maximum value) should be used to rank the vulnerability of the area of interest. Finally, it was mentioned that a kind of validation would be necessary to show that results of SDLM are in principal in agreement with results from monitoring studies. In the end, it was concluded that SDLM for the selection of monitoring wells would be an easier task to start with as it directly connects to a continuation of the SETAC EMAG work, a relative ranking is more important than accurate absolute concentrations and a protection goal would be easier to achieve for this purpose.

The information was given that an initiative from the EU commission (COM) has started to define SPGs needed for future update(s) and/or developments of guidance documents for conducting the environmental risk assessment of pesticides. A first workshop was held on 21\textsuperscript{st} of June with experts from the Member States and EEA-States with the aim to achieve a common understanding on ecosystem services and the proposed EFSA method. The participants of the SDLM workshop agreed that for SPG in groundwater, COM should also take
the initiative together with MS. The regulators network consisting of risk assessors dealing with groundwater monitoring data is also taking up the topic of SPG in groundwater. To develop a framework for a SDLM for the selection of monitoring wells and contextualization it was also discussed to continue the work of the SETAC EMAG group, which may be kicked-off on the Piacenza conference in Sept. 2019, and to find later on a MS or a group of MS to bring the framework to the attention of COM.

Second discussion round
The following points were presented to stimulate the discussion for the second breakout group on regulatory topics:

• How to develop guidance for a harmonised framework (formation of working group, under which umbrella?)
• Which stakeholders should be involved?
• Authority involvement in guidance development (EFSA or some Member States to take the lead)

Information was provided by some participants of the breakout group that it was decided by the “European regulatory network on pesticide groundwater monitoring” to send the SETAC EMAG-GW report (Gimsing et al., 2019; https://link.springer.com/content/pdf/10.1007%2Fs00003-019-01211-x.pdf) as guidance on how to conduct groundwater studies to the commission DG SANTE standing committee SCoPAFF for discussion. This could potentially result in a “taking note” process which means that it would be adopted as it is or the commission could give EFSA a mandate to work on a scientific opinion about this report which would require approx. 3 years.

Therefore, it was argued that SETAC would be an appropriate host also for the initiative of a guidance on SDLM. It was discussed that this could be a two-step process. It would consider in a first step the use of SDLM to support the selection of monitoring wells for dedicated groundwater monitoring studies. In a second step guidance for SDLM as a higher tier modelling method (e.g. Tier 3b) in the FOCUS groundwater scenarios framework should be developed. For this it was again mentioned that a SPGgw would be needed. In this context it was argued that SETAC as a host would provide the advantage that all stakeholders could be on board and could contribute with their experience and expertise to develop a harmonized guidance. The general opinion was that the option to develop a guidance on SDLM as a higher tier modelling method (e.g. Tier 3b) under the umbrella of SETAC is possible and welcomed. Procedurally, in order to make the guidance an official EU guidance for regulatory use, it should go to the SCoPAFF for discussion (i.e. one or more MS have to take the initiative to take the guidance to the attention of COM). The future of the SETAC EMAG-Pest GW report and how it could be managed to establish this report as a guidance could become a precedent case on how to develop guidance under the umbrella of SETAC.

Alternatively, it was discussed that one or a few member states could start an initiative of guidance development as it was for instance the case with CRD (UK) that started the initiative for a “Guidance on how aged sorption studies for pesticides should be conducted, analysed and used in regulatory assessments”. This guidance was commissioned by CRD to research institutes but the lead in steering the process of the guidance development remained with CRD. Stakeholder meetings, contributions and commenting by all stakeholders were possible, including the publication of an EFSA Scientific Opinion (EFSA Journal 2018;16(8):538) following a mandate from the Pesticide Steering Network. The advantage of such an approach would be that a high degree of regulatory acceptance of the included regulatory bodies such as the Commission, EFSA and the MS can be assumed. However, it needs to be taken into account that not all stakeholders could directly contribute in such a working group and that the load of initiating organizing and funding the guidance development would be with one or a few MS authorities.
Finally, it was proposed to discuss the approach that should be followed in a common meeting with the SETAC EMAG-GW working group which should take place as a satellite meeting prior to the Piacenza conference.
Overall Conclusions

Following the breakout sessions all participants reconvened and presented their findings to the larger group. The following topics were discussed:

- Guidance Document
- Model Framework
- Approach
- Regulators

Guidance Document

The key question here is what organization or entities can take the lead on a document detailing the guidance on the harmonization of spatially distributed modelling. Suggestions for a lead organization included:

- SETAC EMAG-Pest GW
  - Option for all parties to participate
- EFSA/MS
  - Funding/resources restrictions were acknowledged
- The group recognized that a smaller subgroup is needed from this group to actually do this work
  - Do we need one model instead of three?

Modelling Framework

With respect to the general modelling framework it was suggested that two versions would be possible each with their own focus and needs. These versions are:

- More refined as higher tier for registration
- Less refined for vulnerability assessment with the intention of monitoring site selection

Approach

During the discussion of the general approach of developing harmonized guidance the following questions were discussed and answered:

- Do we all agree that we should develop a single harmonized guidance for SDLM?
  - YES
- Do we agree that SETAC is a good host for this?
  - Yes
  - However, we recognize that guidance developed under the SETAC umbrella might not really be acceptable by regulatory authorities. It will also depend on how the SETAC EMAG-Pest GW report will be treated by the commission.
- Which member state(s) could possibly take the lead?
  - Several member states were proposed especially NL, AT, DK, Fr? NL indicted some interest but also mentioned that they will not be able to do it alone
  - Regulators network as for SETAC EMAG-Pest GW

Regulators

Some comments and feedback from regulators present at the workshop.

- EFSA Unofficial (might not represent official opinion of EFSA): Good way to continue.
- EFSA looking at landscape level assessment.
• EFSA is not in a position to lead.
• JRC - Can put anything online from the workshop that is needed (presentations and workshop report)
• JRC - Have limitation and resources regarding the support of the initiative. Needs to be seen what can be done.
• JRC can host the databases and tools
• Version control group will meet on 2 September in Piacenza
  ○ VC of databases is on the agenda
• How can the databases and tools be used by regulators and others if everything is going into the cloud?
Follow-up Actions

Availability of presentations and workshop report

- Making it available as PDF
- Should be available for download on JRC site
- Link on PFMODELS or Pesticide models website to JRC site from which documents can be downloaded
- Meeting minutes will be made available and time for review will be given

Follow-up meeting

- Will be held in Piacenza as satellite meeting to the Piacenza conference in the morning of the 3 September
- Will be a joint meeting with the SETAC-EMAG-Pest GW working group
- Invitation will be sent to all participants of this workshop
List of participants

List of participants for the workshop ‘Spatially distributed leaching modelling’ in Ghent on 24 May 2019:

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<thead>
<tr>
<th>First Name</th>
<th>Surname</th>
<th>Affiliation</th>
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