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SPRINT
SUSTAINABLE PLANT PROTECTION TRANSITION

This is a Public Preview of the deliverable. Because of publishing interest the full deliverable is still under embargo.

Integrated fate models to estimate exposure of Ecosystem and Plant for Conventional and Organic farming systems using existing data and new data from the CSS

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Background

One of the main goals of SPRINT is to develop an innovative modelling approach, by integrating plant protection products (PPPs) use with observed concentrations and exposure levels and linking fate and transport of PPPs to direct and indirect health impacts, resulting in a paradigm shift in this field of research. This has short- and long-term implications for agri-food industry, PPPs' users, regulatory bodies, and society as a whole. Inclusion of specific PPP transport pathways currently ignored in existing models, such as aerial transport of pesticide-containing soil particles by wind and tillage erosion, will provide better insights into the environmental fate of pesticide residues and exposure levels to ecosystem, plant, animal and human (EPAH) Toxic-kinetic models will be refined using data from laboratory-based human volunteer studies for model calibration and biomonitoring data from CSS to test how well the models reflect real-life conditions.

Working Package (WP) 3, in particular tasks 3.2 and 3.3, aims to complement the fate and transport and the exposure data from the systematic literature review with the data collected from the Case Study Sites (CSS), enhancing the verification and the validation of the exposure assessment for ecosystems, animals and humans. In this deliverable just the ecosystem and plant assessments are taken into consideration. Animal and human assessments are taken into consideration in deliverable D3.3" Integrated exposure model to estimate exposure of animals and humans for conventional, integrated pest management and organic farming scenarios using models calibrated with data from the CSS", with due date also of 31 August 2023.

Therefore, the purpose of this document is to i) assess the fate and transport of PPPs used in three CSS, Portugal, the Netherlands and Denmark, one for each regulatory zone according to Regulation (EC) No. 1107/2009 (figure 0.1.), in soil, water and air; ii) verify the models performance and assumptions made during the development of the scenarios by comparing simulated data with monitoring data from CSS; iii) validate the performance of the wind erosion module, developed within SPRINT, by comparing the simulated data with the monitoring data from the two modelling reference CSS, Portugal and The Netherlands; and finally iv) assess the plant exposure and compare the simulated results with the monitoring results collected in the three CSS. As mentioned in the working document *"Additional Monitoring plan for exposure models verification"* the two countries Portugal and The Netherlands have been selected as reference modelling CSS and additional environmental samples were collected to ensure the verification of exposure model simulations.

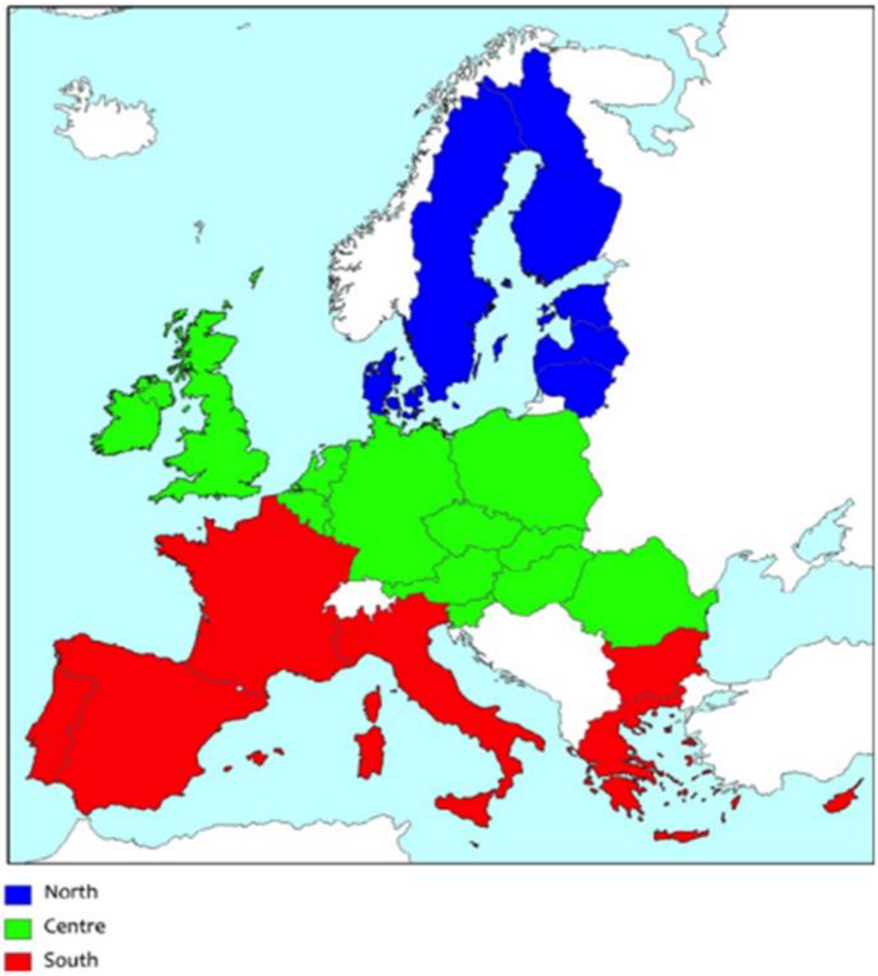

Figure 0.1. The three regulatory zones according to Regulation (EC) No. 1107/2009 – EFSA

This document reflects the selection made previously in the Milestone 4 *"Model chains defined, including input and output relationships"* concerning the model chain, with the input and output connections for the assessment of the fate of pesticides in soil, surface water and sediments, air outdoor and dust indoor and of the exposure of aquatic and soil organisms (figure 0.2.).

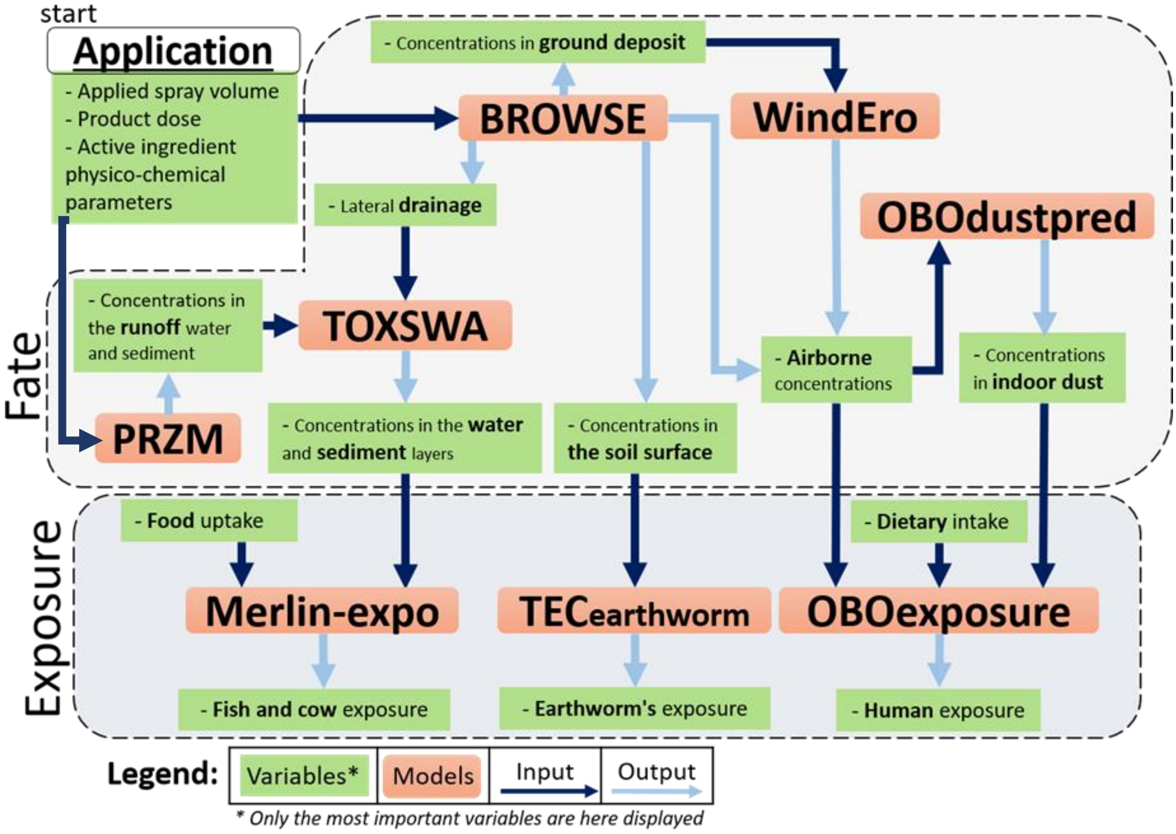

Figure 0.2. – Model chain, connections and most relevant inputs and outputs, as described in the Milestone 4. Note: "Start application" represents the input for both PRZM and BROWSE.

Main results and conclusions

In this deliverable, D3.2, we studied the fate and transport of some of the pesticides used in three CSS, two reference CSS PT and NL, and DK, in soil, surface water, sediment, air and crops. Furthermore, the simulated concentrations were then used to assess the exposure of aquatic organisms, plankton, invertebrates and fish, and soil organisms, earthworms, to the pesticides selected. Finally, the simulated results were compared with the monitoring results to assess the appropriateness of the model calculation. The three countries were selected as representative counties for each regulatory zone according to Regulation (EC) No. 1107/2009. In the two Reference CSS additional monitoring campaigns were undertaken to allow a higher amount of data for model performance verification. The pesticides selected for the simulations were selected based on three criteria: (i) real application in the field, (ii) presence in the environmental matrices under study and (iii) physicochemical properties suitable to ensure the possible presence in the matrix of interest.

Even if an identical assessment approach considering the same environmental matrices was scheduled for the two reference CSS PT and NL, the territorial reality and the data collected and used as input for the models didn't allow it. Furthermore, as DK CSS was not selected as reference CSS no air assessment was undertaken. Figure 0.3 shows the matrices considered in each country.

In total, in the three CSS and all matrices considered, 22 PPPs and 5 different crops (grape in PT, potatoes, sugar beet and onions in NL and spring barley and winter wheat in DK) were considered for the assessment. 11 out of the 22 PPPs were considered just for the particle phase assessment in NL CSS.

Considering the surface water assessment, the simulated results in **PT CSS** showed a very low exposure of water bodies with PECsw values lower than EQS, mainly due to the low rainfall in the post-application period resulting in low runoff and a distance of more than 30 meters between the water body and the application plots, which determines a mitigation of the drift of greater than 90%. Furthermore, the estimates through the FOCUS models have been successfully integrated in MERLIN-Expo model for an assessment at a larger scale. The modelling exercise allowed assessing the contribution of the different plots to the contamination of the main river in the catchment. However, several limitations of the application of Merlin-Expo were observed due to the limited information about the real river structure and miss of important processes in the model. Indeed, dispersion and re-suspension of sediment are not considered by the model. Furthermore, no information about the use of the three fungicides in other fields located near the considered water bodies were available. Therefore, it would be advisable to carry out a more in-depth

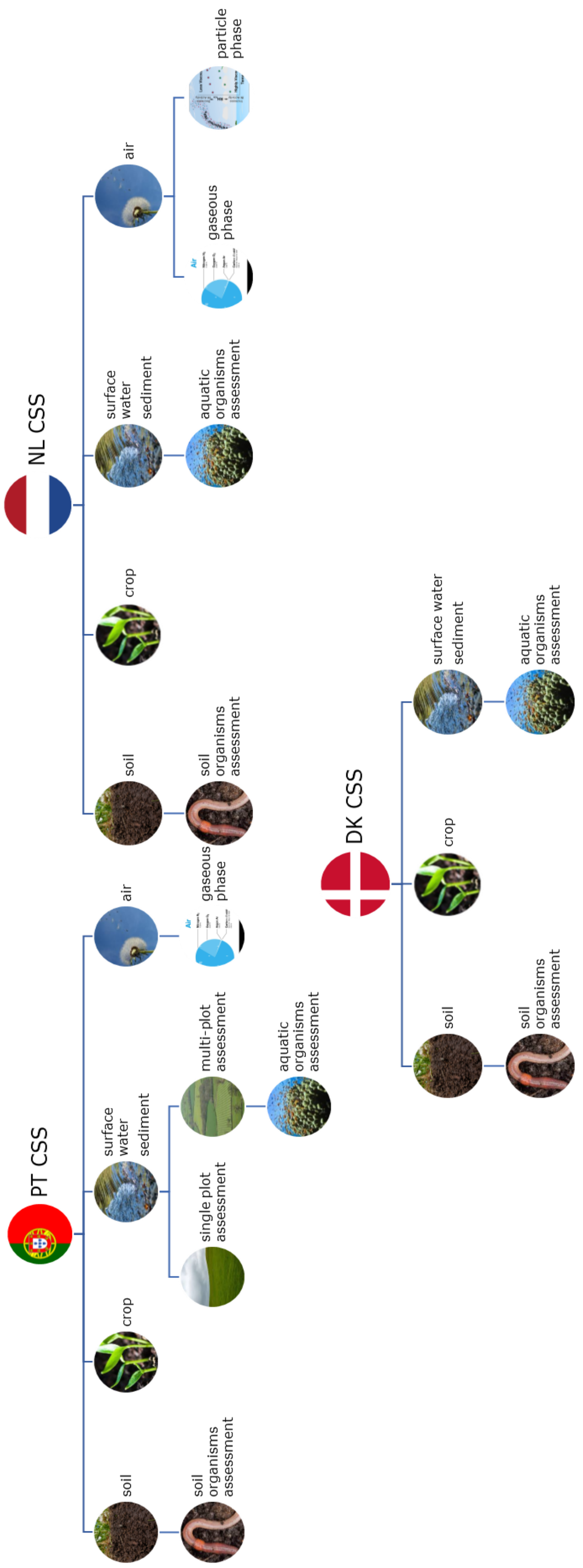

Figure 0.3 Matrices taken into consideration for the modelling assessment in PT, NL and DK

investigation that considers the different fields adjacent to the Cértima and its tributary, the real river structure and a river model that considers the afore mentioned processes to verify the impact of the different fungicides in water bodies in a more precise and continuous time frame. **For NL CSS**, the PEC_{SW} calculated by the models showed a significant exposure of the water bodies to the two a. ss considered, acetamiprid and mandipropamid, with values during the entire simulation period (up to 28 days after PPPs application) higher than EQS. The main route of entry is spray drift. In FOCUS models, runoff only occurs when daily precipitation is higher than 2cm (20mm). Since no significant precipitations occurred the first days after the application of the two pesticides, runoff contribution is negligible. However, the PECsw results obtained should be considered as very preliminary results indicating a certain exposure of water bodies to the PPPs used in the agricultural fields of the area under study since in the assessment just three fields were considered, without considering that other fields in the watershed could have been treated and without considering the complex hydrographic scheme of the watershed.

For DK CSS, the PEC_{SW} calculated by the models showed a moderate exposure of the water bodies to the two a.s.s considered, diflufenican and prosulfocarb, right after the application, with values higher than the EQS. However, already from the first day after the application the concentrations decreased below the afore mentioned standard. The main route of entry in surface water was spray drift at the date of application. Loadings from surface runoff were negligible because a runoff event in PRZM model can be triggered only if the daily rainfall is above 20mm, which wasn't the case.

In general, for surface water assessment in all three CSS when comparing the simulated results with the monitoring results, an overestimation of simulations of maximum two orders of magnitude was observed.

However, when using these simulated results for the estimation of **concentrations in invertebrates and fish,** the predicted results indicate that their consumption would not lead to values above the acceptable daily intake established for humans **for PT and NL CSS**. **In DK CSS**, for the herbicide prosulfocarb based on its current established ADI and considering the simulated results, already a small consumption (above 13 grams) of a given invertebrate (e.g. crawfish or sea urchin) would lead to an estimated daily intake over the ADI (assuming human bodyweight of 70). It is important to stress that the model takes an average invertebrate weight, and this can affect predicted concentration based on each species weight. For diflufenican, no risk for human consumption is foreseen at simulated concentrations.

Considering the soil assessment, in general, the simulated PECsoil in **PT CSS** resulted lower than the monitored values for all three compounds considered. In one single case dimethomorph show PECsoil values almost 5 times higher than the monitored values.

Without having background values in the soil of the three plots, it is difficult to explain the significant discrepancies between the simulated and the monitored results.

For NL and DK CSS an overestimation of one order of magnitude of the simulated PECsoil was observed. It must be considered that the PECsoil were calculated with FOCUS Soil Calculator, therefore are worst case values considering only the degradation in soil without considering other losses (mainly leaching).

The PECsoil were further used to calculate the **toxicity to exposure ratio (Ter)** for acute and long-term **exposure for earthworms**. **For all three CSS** the TER values indicate there is low risk for earthworms. However, for metalaxyl-M, used in PT CSS, several studies indicated toxicity effects at low concentration. Indeed, when recalculating the exposure-toxicity ratio (TER) with genotoxic effect as an outcome the values indicated that over a continuous exposure to metalaxyl-M DNA damage would likely occur.

Considering the air assessment in gaseous phase, the simulated PECair were all the time above the monitored values. If for **PT CSS** the overestimation was up to one order of magnitude, which is not bad, for **NL CSS** the models overestimated up to five orders of magnitude the PPPs measured concentrations.

The **wind erosion model** developed within SPRINT, SWIPPE, and applied just for **NL CSS** seems to perform well considering that most modelled values follow the same trend as measured values, even when differences are large. In most cases, the model predictions were close to the true mean. However, there is a larger uncertainty surrounding some of the input data and also background values of particle-phase PPPs (i.e. other sources). Despite these limitations the model still performed well, given that the largest differences were in the order of nanograms.

Finally, the **estimated concentrations at crop canopy** together with the total quantities of pesticides applied in the CSS, were used to calculate the percentage of pesticides in crops with respect to the total quantities applied. The results show values ranging from 18% to 55.5%.

Overall, the models used for the different assessments performed well considering that in most of the cases the difference between the simulated and the monitored concentrations were of maximum two orders of magnitude and that the largest differences were in the order of nanograms. The appropriateness of the model calculation can be either assessed by modelling statistics or simulation graphics. The large amount of data, however, enhances the use of comprehensive model deviation indicators. However, in our case, the very low amount of experimental data (beside the concentrations in the air), which was almost all the time just one sampling time (useful for comparison), doesn't allow the use of model deviation indicators.

Limitations of modelling exercise

The outputs of the present modelling exercise were highly influenced by the limited data available as input for the models, collected from the three CSS, and in some cases by the miss of important processes in the models and tools.

One of the most important limitations related to the data used as input for surface water, soil and plant assessments is the availability of suitable weather data. Indeed, in the Milestone 3 "Model data requirements identified" we highlighted the need of weather data from weather stations close to the fields where the PPPs are applied, giving as maximum distance 5 km. However, for NL and DK CSS we have used for the assessments data collected by weather stations located at 7, 12, 27 and 73 km away. This made the prediction of drift during the application and of run-off events after application highly questionable and influenced the predicted PECsw and PECsed in the water bodies. Furthermore, for PT CSS the weather data collected didn't covered the entire application period of PPPs and for some months data from the most recent available months was used. This may have also influenced the PECsw and PECsed values in PT CSS. Use of proper climatic conditions may also have influenced the PECsoil values, as processes as degradation are highly dependent on the temperature.

Concerning the PECair in both gaseous and particulate phases, even if the weather stations in both PT and NL CSS were near the fields, we measured wind speed and collect data at/from one single point. PPP spray, wind speed and wind erosion are highly variable in space. Therefore, this may have influenced the predicted values, and this variability is very difficult to account for.

Furthermore, for the scenario development very limited data about the surface water bodies hydrology and structures were available. Indeed, in most of the cases one single streamflow measurement was available. Therefore, using a single streamflow value in a highly variable stream which dries up in summer, like in PT CC, or in a human-managed drainage ditch system, like in NL CSS, may have significantly influenced the predicted water concentrations, even if the loads from filed or during application were correctly predicted. Continuous streamflow measurements would have been useful to properly assess the performance of the used models.

However, in some cases important processes influencing the fate and transport were not considered in the models. This is the case of river model in MERLIN-Expo tool that doesn't consider dispersion and re-suspension of sediment and of FOCUS Soil calculator that doesn't consider losses by leaching. Therefore, alternative models should be used to overcome these limitations.

Concerning the evaluation of models' prediction performance, several limitations were individuated. Firstly, we could not account for PPPs used in other fields during the simulated periods. This would account for model underestimation when comparing with measured data. Secondly, beside the PECair assessment, a very low amount of experimental data (one single sampling time) was available and useful for comparison between predicted and monitored results. Indeed, in most of the cases the sampling campaigns didn't follow the application PPPs calendar, even if an additional monitoring plan was developed to support modelling exercise. Finally, no useful background values were available.

However, beside all these limitations, overall, the models performed well considering that in most of the cases the difference between the simulated and the monitored concentrations were of maximum two orders of magnitude and that the largest differences were in the order of nanograms. The exception was PECair prediction in gaseous phase where the differences between the predicted and the monitored values were up to five orders of magnitude.

All the FOCUS models and tools used in the present modelling exercise are authorised for regulatory purposes while PEARL-OPS, present in BROWSE, and MERLIN-Expo are models often used for environmental assessments. Based on the outputs obtained we can confirm the robustness of FOCUS models and tools for the assessment of PPPs fate and transport in soil and surface water, while we highlight the limitation of MERLIN-Expo for surface water large scale assessment and of PEARL- OPS for PECair predictions.

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