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Modelling the fate of veterinary compounds in groundwater and surface water using the FOCUS models

Harmonisation of input parameters and interpretation of results

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On behalf of the German Environment Agency

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For authorization procedures, the guidelines of the European Medicines Agency are to be followed.

Abstract: Modelling the fate of veterinary compounds in groundwater and surface water using the FOCUS models

In this project harmonised input parameters for the FOCUS groundwater model PEARL and the FOCUS Surface waters models (SWASH, PRZM, MACRO, TOXSWA) were suggested and it was assessed whether the currently used options and parameters are still valid. Furthermore, recommendations were developed about how the models could be used and how their results could be interpreted in the risk assessment for veterinary medicines. The results of this project can aid in future the discussions on guidance documents for the ERA of veterinary medicines. The report also includes a manual for performing FOCUS simulations. It was also investigated in how far FOCUS tools could be used to evaluate mitigation options for veterinary compounds.

Following results were obtained:

- In addition to Okehampton Hamburg, Jokioinen and Piacenza scenarios may be as well of relevance for the assessment of PEC groundwater.
- The crop maize should be additionally considered in the risk assessment for manure applications.
- The crop grass/alfalfa scenario should be used for a scenario when animals are kept under outdoor conditions. It is recommended to divide the application over the period of treatment and to use an incorporation depth of 0 m.
- Technically, risk mitigation could be performed for run-off scenarios using the FOCUS SWAN routine. The software uses vegetated buffer strips as mitigation option. However, results would only be valid for locations with vegetated buffer strips and are thus not applicable in the general risk assessment.
- In case sorption are pH dependent and not correlated to the organic carbon content, it is recommended to use worst-case selections (e.g. minimum sorption constants).

Kurzbeschreibung: Modelling the fate of veterinary compounds in groundwater and surface water using the FOCUS models

In diesem Projekt wurden harmonisierte Eingabeparameter für das FOCUS Grundwassermodell PEARL und die FOCUS Oberflächenwassermodelle (SAWSH, PRZM, MACRO, TOXSWA) vorgeschlagen und es wurde analysiert, ob die aktuell verwendeten Einstellungen und Parameter noch sinnvoll sind. Außerdem wurden Empfehlungen zum Einsatz und zur Interpretation der Ergebnisse im Rahmen der Risikobewertung von Tierarzneimitteln zusammengestellt. Die Ergebnisse dieses Projekts können zukünftige Diskussionen zu Leitfäden für die Risikobewertung von Tierarzneimitteln unterstützen. Der Bericht enthält auch ein Handbuch zur Durchführung von FOCUS Berechnungen. Es wurde auch untersucht inwieweit die FOCUS Programme für Risikominderungsmaßnahmen für Tierarzneimittel eingesetzt werden können.

Folgende Ergebnisse wurden erzielt:

- ► Hamburg, Jokioinen und Piacenza können zusätzlich zu Okehampton als relevante Szenarien für die Risikoabschätzung für Grundwasserkonzentrationen eingesetzt werden.
- ► Für die Risikoabschätzung von Tierarzneimitteln bei Gülleapplikationen sollte zusätzlich die Kultur "Mais" berücksichtigt werden.
- ► Die FOCUS Kultur "Grass/Alfalfa" sollte als Szenario eingesetzt werden, wenn Tiere unter Freilandbedingungen gehalten werden. Die Applikationsrate sollten über die Zahl der Behandlungstage aufgeteilt werden. Es sollte eine Einarbeitungstiefe von 0 cm simuliert werden.
- ► Der Einfluss von Risikominderungsmaßnahmen bei Runoff könnte grundsätzlich mit dem Computerprogramm FOCUS SWAN berechnet werden. Die Software verwendet bewachsene Pufferstreifen als Minderungsmaßnahme. Allerdings wären die Ergebnisse nur gültig für Standorte mit entsprechenden Pufferstreifen und nicht allgemein in der Risikobewertung anwendbar.
- ► Es wird empfohlen, Worst-Case-Einstellungen zu verwenden, wenn die Sorption einer Substanz nicht mit dem organischen Kohlenstoffgehalt, sondern mit dem pH-Wert korreliert. Das bedeutet, es sollte in diesen Fällen die minimale Sorptionskonstante verwendet werden.

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List of abbreviations

EFSA	European Food Safety Authority
EMA	European Medicines Agency
FOCUS	Forum for the Coordination of pesticide fate models and their use (organisation that developed the FOCUS groundwater and surface water models that are used as higher tier options in the risk assessment of veterinary compounds.
GW	Groundwater
Kfoc	Kfoc (unit L/kg) is the Koc normalized Freundlich adsorption coefficient.
Koc	The adsorption coefficient Koc (unit L/kg) is the ratio of the substance concentration in soil related to the substance concentration in the water phase related to the organic carbon content in soil.
Kom	The adsorption coefficient Kom (unit L/kg) is the ratio of the substance concentration in soil related to the substance concentration in the water phase related to the organic matter content in soil.
MACRO	MACRO is a physically-based one-dimensional numerical model of water flow and reactive solute transport in field soil. It is part of the FOCUS SW package and used to calculate drainage entries into surface water
PAT	Pesticide Application Timer (internal tool in the FOCUS SWASH package to avoid unrealistic weather conditions for application dates)
PEARL	PEARL is an acronym of Pesticide Emission Assessment at Regional and Local scales. It is a one-dimensional numerical model of pesticide behaviour in the soil-plant system and used for the assessment of groundwater concentration.
PEC	Predicted environmental concentration
PRZM	Pesticide Root Zone Model (numerical model that is part of the FOCUS SW package and used to calculate run-off and soil erosion after storm events)
SW	Surface water
SWAN	Surface Water Assessment Enabler (User shell for performing additional risk assessment for FOCUS SW scenarios)
SWASH	Surface Water Scenario Help (User shell for performing FOCUS SW simulations)
TOXSWA	Toxic substances in Surface Waters (numerical model that is part of the FOCUS SW package and used to calculate surface water concentrations)
VFSMOD	Vegetative Filter Strip Modelling System (numerical model that is part of the FOCUS SWAN package and used to mitigate the risk caused by run-off and soil erosion)

Summary

Background

In this project harmonised input parameters for the FOCUS groundwater model PEARL and the FOCUS Surface waters models (SWASH, PRZM, MACRO, TOXSWA) are suggested and it is assessed whether the currently used options and parameters are still valid. Furthermore, recommendations are developed about how the models could be used and how their results could be interpreted in the risk assessment. The results of this project are compiled in a way that it could serve as a base for a future manual for authorities and applicants when performing FOCUS simulations within the risk assessment. It is also investigated in how far FOCUS tools could be used to evaluate mitigation options for veterinary compounds.

The risk assessment for veterinary compounds is performed because they could have adverse effects on ecosystems in the environment. Therefore, before authorisation, an environmental risk assessment has to be conducted. An important part of the risk assessment for veterinary medicines is the evaluation their exposure.

The risk assessment consists of several tiers. The initial calculation (Tier A assessment) follows straightforward equations using default values and information from the product literature. The refined calculation of groundwater concentrations for veterinary products is done based on the computer software FOCUS PEARL. Respective surface water simulations are performed using a software package with three different computer models (MACRO, PRZM, TOXSWA) connected by the shell SWASH.

The FOCUS scenarios were originally developed for pesticides. This is the reason why the shell and some of the input parameters incl. default values are not always in line with the needs in the risk assessment for veterinary compounds. However, this does not discredit the application of these models for veterinary compounds. The assumptions used in the model are valid also for other compounds than pesticides.

Compared to the straightforward equations used for the Tier A assessment, FOCUS developed higher tier numerical models with detailed environmental scenarios which describe realistic worst-case situations for major agricultural areas in Europe (FOCUS 2000). As surrogate for ground water concentrations FOCUS uses percolate concentrations at a depth of 1 m. This assumption can be considered a conservative approach. The idea of the groundwater scenarios was to combine the 80th spatial percentile (the soil scenarios) with the 80th temporal percentile (calculated based on a weather series of 20 years). That should result in an overall 90th percentile.

With regard to surface water FOCUS defined three entry routes (spray drift, run-off/erosion and drainage). Spray drift is not relevant for veterinary compounds since the substances are incorporated (no-drift situation). Run-off is overland flow occurring after heavy rainfall followed by the transport of substances into surface water via the solved phase. Together with run-off also suspended particles are transported into surface water bodies. Therefore, also substances with high sorption constants which do not appear in the water phase could be transported into surface water bodies via the sediment particles (soil erosion). The third entry route into surface water is transport via drainage system. Here only the water phase is considered (no sediment).

FOCUS defined three different surface water bodies: ponds, ditches, and streams. Incoming water, caused by run-off or drainage events, is always diluted with water in the respective receiving water system. Further dilution is caused by the upper water catchment area. Maximum concentrations are often relatively fast reduced by transport out of the system. Basically, also the FOCUS surface water scenarios aim at the overall 90th percentile for their simulations but the

construction of the scenarios is less explicit. Especially the short simulation period of only a single year was often criticised which may have led to the formation of EFSA's FOCUS repair working group that recently recommended a simulation period of 20 years also for FOCUS surface water simulations (EFSA 2020). Unfortunately, the FOCUS surface water models had not been updated at the time this report was written.

Relevance of the FOCUS groundwater locations

The FOCUS groundwater assessment is originally based on 9 different locations distributed over Europe. They are intended to represent major agricultural areas. According to the current EMA guideline only a single scenario (Okehampton) is used in the risk assessment for veterinary compounds (EMA 2005). However, new studies point out that in contrast to (EMA 2005) there are major agricultural areas with high intensity of livestock production also in regions where other FOCUS scenarios are representative for the application of veterinary compounds. In order to check the relevance of the FOCUS groundwater scenarios simulations with the most recent version of FOCUS PEARL (which is 5.5.5) are performed for 48 (hypothetical) veterinary compounds with Kfoc in the range of 1 L/kg to 3000 L/kg and DegT50 in the range of 1 d to 300 d. All FOCUS scenarios where the crop 'winter cereals' is cultivated were considered. The application pattern was 1 kg/ha 14 days before crop emergence. Parallel calculations were also done with the initial Tier A assessment. The FOCUS model always calculates concentrations below respective values of Tier A. With regard to the influence of sorption and degradation on the simulated concentrations, the following results were found: Decrease of sorption and of degradation always leads to an increase of the concentration in groundwater. Assuming the compound has a Kfoc of or above 3000 L/kg, the model does not simulate any concentrations for compounds with DegT50 up to 300 d independent of the FOCUS location. The evaluation additionally showed that Okehampton represents a reasonable worst-case scenario for many compounds. However, the results also showed that for low sorbing compounds with Kfoc below 30 L/kg other scenarios (e.g., Hamburg, Jokioinen) would be a better choice. Piacenza (as a Mediterranean location) also shows higher concentrations than Okehampton for this type of compounds. Therefore, in addition to Okehampton, Hamburg, Jokioinen, and Piacenza may be as well of relevance for the assessment of PECgw.

Alternative maize scenario for manure applications

In order to check the impact of using the alternative maize scenario instead of winter cereals the same (hypothetical) veterinary compounds were used as before. Also, the same application pattern was considered (1 kg/ha 14 days before crop emergence).

With regard to groundwater, it was concluded that that significantly lower concentrations are simulated in maize than in winter cereals for short living compounds (half lives up to 30 days). Background is the different application season (spring in maize, autumn in winter cereals). The dominant season for leaching is in autumn/winter period. When applied in spring most of the applied compounds were already degraded before autumn was reached when they were applied in spring. However, if the compounds were more persistent (half-life above 100 days) the difference between autumn and spring application became less relevant and occasionally even higher concentrations are simulated in maize than in winter cereals (e.g., compounds with Kfoc = 100 L/kg at Sevilla).

A similar trend was found for surface water: Most of the simulations resulted in lower concentrations than in winter cereals for all kind of compounds. There was, however, a significant exception from this trend: The R4 stream scenario in maize always resulted in higher concentrations than R4-stream when winter cereals was cropped. The extreme range was explained by the different season of application. With the present weather data R4 applications in spring represent worst-case conditions rather than application in autumn. This observation could be also a consequence of the short simulation period of only a single year and the situation could change after extending the simulation period to 20 years (next update of the models).

It was finally concluded that since maize is currently an important crop for the application of manure it would make sense to consider maize in the risk assessment for veterinary compounds when assessing the leaching of these substances to groundwater and surface water.

New scenario for animals kept under outdoor conditions

There are currently no recommendations how to use the FOCUS models when animals are kept under outdoor conditions on pastures. Nevertheless, FOCUS simulations could be also performed for this situation assuming some input parameters are adapted. Similarly, as for the intensively reared animals under indoor conditions, the initial concentration in soil should be the base for the calculation. FOCUS models are using a daily time step. It is therefore recommended to distribute the application rate (calculated based on the initial soil concentration) over the period of treatment. If, for example the animals are treated over a period of 5 days one fifth of the total application rate should be applied over five following days. That would result in a more realistic application pattern than the total amount on one day. With regard to other input parameters, it is recommended to consider FOCUS crop grass/alfalfa with fixed applications dates beginning on March 1 or October 1. Application should be made with an application depth of 0 m. Results of FOCUS groundwater scenarios for a compound with Kfoc=300 L/kg and a DegT50 in soil of 100 d when in 1 kg/ha was distributed over 8 days in March showed that significantly lower concentrations are to be expected than for winter cereals and maize, at least for this compound. The general trend with regard to the ranking of concentrations for the different locations is similar. Though the results may be different for different compounds it was concluded that the FOCUS grass/alfalfa scenario gives reasonable results and could be used for the risk assessment when animals are kept under outdoor conditions.

Consideration of risk mitigation methodologies

Originally, the FOCUS surface water models only consisted of three steps without any additional risk mitigations methodologies (FOCUS 2001). However, for the risk assessment of pesticides it was necessary to include a final step where additionally risk mitigation methodologies can be considered. Basically, drift mitigation (buffer zones, special nozzles) and run-off mitigation (vegetated buffer strips) are considered at the final step. Drainage mitigation options are not offered. For veterinary compounds, only run-off mitigation is of relevance since for all FOCUS SW simulations the application type "granular application" is used which assumes no drift entries into surface water.

The final step of the refined calculation could be easily performed using the software SWAN if standard FOCUS simulation results are available. This software supports the user in modifying the existing output of PRZM (i.e., run-off entries) for the simulation. SWAN also updates the TOXSWA input files so that the surface water model will use the modified PRZM output. It is currently planned to establish SWAN as an official FOCUS model at the FOCUS website.

The EMA reflection paper on risk mitigation measures (EMA 2012) mentions minimum distances to surface water when spreading manure from treated animals as a potential measure. This measure is the same as what is currently done in the final step of the FOCUS surface water risk assessment with SWAN. Thus, it would be technically possible to further refine the concentration in surface water for those locations where vegetated buffer strips of at least 10 m exist.

The EMA reflection paper classifies this risk mitigation measure as "not under control of the veterinarian or animal owner" and does therefore not recommend it. Although a recalculation of exposure would be technically possible for certain locations, the risk cannot be reliably mitigated on an EU wide level.

Modelling ionising substances

Many veterinary compounds are ionising substances. The consequence is that the standard assumption of strong correlation of organic carbon content in soil and sorption does not work. Guidance how to consider this type of substances in the risk assessment is given in an EMA questions and answers document (EMA 2018). While in the initial assessment the lowest Koc is to be used, for higher tier assessment it recommends using the most appropriate adsorption coefficient.

The FOCUS GW report (FOCUS 2009) gives advice how to consider substances where sorption is dependent on pH in soil. PEARL is able to consider the pH-dependency by assuming that the dependency is caused by different fractions of the ionised and the non-ionised form dependent on the pH in soil. The user has to enter the "pure" Koc for both forms. For estimating the fraction dependent on the pH the pKa is additionally needed. The pKa determines at which pH the distribution between the two forms is equal.

Though this procedure is a valid transformation of the behaviour of ionising substances to other pH values it may nevertheless violate the original definition of the FOCUS locations as worst-case scenarios. Background is that the soil pH values were never used as a selection criterion in the development and may therefore also not represent worst-case conditions (as e.g., organic carbon contents or the climatic conditions) in soil. Therefore, as a simple, practical and conservative strategy also a simulation based on the worst-case sorption constant in the laboratory study (i.e., the minimum value) could be used for the risk assessment. The same worst-case strategy could be considered also when the sorption constant is correlated to other soil parameters (e.g., the clay content) or the DegT50 is pH-dependent.

The FOCUS SW report (FOCUS 2001) does not discuss the problem of ionising substances. Independent whether sorption is found to be correlated with organic carbon in soil or whether Kfoc/DegT50 are pH-dependent the mean values should be considered for the simulations. However, it may be more appropriate to consider worst-case selections (e. g., minimum Kfoc, maximum half-life) in case the respective parameters are clearly correlated to the pH in soil.

Manual

The final chapter of the report contains a detailed manual explaining the practical use of FOCUS PEARL, FOCUS surface water, and FOCUS SWAN for veterinary medicines.

Zusammenfassung

Hintergrund

In diesem Projekt werden harmonisierte Eingabeparameter für das FOCUS Grundwassermodell PEARL und die FOCUS Oberflächenwassermodelle (SAWSH, PRZM, MACRO, TOXSWA) vorgeschlagen, und es wird analysiert, ob die aktuell verwendeten Einstellungen und Eingaben noch sinnvoll sind. Außerdem werden Empfehlungen zum Einsatz und zur Interpretation der Ergebnisse im Rahmen der Risikobewertung von Tierarzneimitteln aufgeführt. Die Ergebnisse dieses Projekts sind so zusammengestellt, dass sie als Basis für ein zukünftiges Handbuch für Anwender aus Behörden und Industrie dienen können, wenn FOCUS Simulationen im Rahmen der Risikoabschätzung von Tierarzneimitteln gemacht werden sollen. Schließlich wird auch untersucht, inwieweit die FOCUS Programme für Risikominderungsmaßnahmen für Tierarzneimittel eingesetzt werden können.

Die Risikoabschätzung von Tierarzneimitteln wird durchgeführt, weil die Stoffe ungünstige Effekte auf Ökosysteme in der Umwelt haben können. Deshalb wird vor ihrer Zulassung eine Umweltrisikobewertung durchgeführt. Ein wichtiger Teil dieser Abschätzung ist die Untersuchung der Exposition.

Die Expositionsabschätzung besteht aus mehreren Stufen. Die Eingangsberechnung (Tier A) verwendet Gleichungen mit Standardwerten und Daten aus der Produktliteratur. Die verfeinerte Berechnung für Grundwasserkonzentrationen der Tierarzneimittel wird auf der Basis des Computermodells FOCUS PEARL durchgeführt. Berechnungen für Oberflächenwasser erfolgen mit einem Softwarepaket aus drei verschiedenen Computermodellen (MACRO, PRZM, TOXSWA), die über die Benutzeroberfläche SWASH gekoppelt sind.

Die FOCUS-Szenarien wurden ursprünglich für Pestizide entwickelt. Dies ist der Grund dafür, dass die Benutzeroberfläche und einige Eingabeparameter nicht immer mit den Anforderungen der Risikoabschätzung für Tierarzneimittel übereinstimmen. Das bedeutet aber nicht, dass die Modelle für Tierarzneimittel ungeeignet sind. Die Annahmen der FOCUS-Modelle sind grundsätzlich auch gültig für andere Substanzen als Pestizide.

Im Vergleich zu den einfachen Gleichungen der initialen Stufe (Tier A) wurden von FOCUS höherwertige numerische Modelle mit detaillierten Umweltszenarien entwickelt, die „realistic worst-case“ Situationen für größere landwirtschaftliche Gebiete darstellen (FOCUS 2000). Als Stellvertreter für Grundwasserkonzentrationen werden von FOCUS Perkolatkonzentrationen in einer Tiefe von 1 Meter verwendet. Dies kann als konservative Annahme angesehen werden. Die Idee der Grundwasserszenarien war ein 80. Flächenperzentil (Bodenszenario) mit einem 80. zeitlichen Perzentil (basierend auf Wetterserien über 20 Jahre) zu verknüpfen. Diese Strategie sollte zu einer Gesamtperzentile von 90% führen.

Für das Oberflächenwasser definierte FOCUS drei verschiedene Eintragspfade (Spraydrift, Abschwämmung (Runoff)/Erosion und Dränage). Spraydrift ist für Tierarzneimittel nicht relevant, da die Substanzen eingearbeitet werden. Runoff ist oberflächlich ablaufender Wasserfluss nach Starkregen gefolgt von einem Transport der Tierarzneimittel über die Wasserphase. Gleichzeitig mit dem Runoff gelangen auch suspendierte Bodenpartikel in das Oberflächengewässer. Deshalb können auch stark sorbierende Substanzen, die nicht in der reinen Wasserphase auftauchen, über die Sedimentphase in das Gewässer gelangen (Bodenerosion). Der dritte Eintragspfad ins Gewässer stellt Transport über Dränagesysteme dar. Hier wird nur die Wasserphase berücksichtigt, kein partikelgebundener Transport.

FOCUS hat drei verschiedene Gewässertypen definiert: Teiche, Gräben und Bäche.

Zusätzliches Wasser, verursacht durch Runoff- oder Dränageereignisse wird immer durch das Wasser im Gewässer verdünnt. Weitere Verdünnungen entstehen durch das obere Wassereinzugsgebiet. Maximale Substanzkonzentrationen werden häufig relativ schnell durch Transport aus dem System reduziert. Grundsätzlich zielen auch die FOCUS Oberflächenwasserkonzentrationen auf das 90. Gesamtperzentil, allerdings ist die Konstruktion der Szenarien weniger explizit.

Vor allem die kurze Simulationsperiode von einem Jahr wurde oft kritisiert. Dies mag zur Bildung der „EFSA FOCUS Repair“ Arbeitsgruppe geführt haben, die kürzlich empfohlen hatte, eine Simulationsperiode von 20 Jahre auch für die Oberflächenwasserszenarien zu verwenden (EFSA 2020). Leider wurden die FOCUS Modelle zum Zeitpunkt dieses Berichts noch nicht aktualisiert.

Relevanz der FOCUS Standorte (Kompartiment Grundwasser)

Die FOCUS Bewertung für Grundwasser basiert ursprünglich auf 9 verschiedenen über Europa verteilten Standorte. Sie wurden ausgewählt, um größere landwirtschaftliche Gebiete zu repräsentieren. Jedoch wird entsprechend der aktuellen EMA Richtlinie nur ein einziges Szenario (Okehampton) für die Risikoabschätzung für Tierarzneimittelprodukte verwendet (EMA 2005). Allerdings zeigen neue Studien, dass im Unterschied zu (EMA 2005) größere landwirtschaftliche Gebiete mit einer hohen Dichte für Tierproduktion auch in Regionen existieren, für die andere FOCUS-Szenarien repräsentativ sind.

Um die Relevanz der anderen FOCUS Grundwasserszenarien zu überprüfen, wurden mit der neuesten Version von FOCUS PEARL (Version 5.5.5) Simulationen mit 48 hypothetischen Tierarzneimitteln durchgeführt. Der Kfoc der Substanzen wurde im Bereich von 1 L/kg bis 3000 L/kg variiert, der DegT50 im Bereich von 1 bis 300 d. Für alle Rechnungen wurde die Kultur Wintergetreide verwendet. Das Applikationsmuster war eine Aufbringungsmenge von 1 kg/ha 14 Tage vor dem Feldauflauf. Parallele Berechnungen wurden zusätzlich mit den Gleichungen der Stufe A (Tier A) durchgeführt. Es zeigte sich, dass die FOCUS Modelle grundsätzlich Konzentrationen unterhalb der Stufe A Abschätzung berechnen. Bezogen auf den Einfluss von Sorption und Abbau wurden folgende Ergebnisse erzielt:

Abnahme von Sorption und Abbau führten immer zu einem Anstieg der Grundwasserkonzentration. Substanzen mit einem Kfoc von 3000 L/kg führten grundsätzlich zu keinem Eintrag ins Grundwasser, selbst wenn für die Halbwertzeit 300 Tage angenommen wurde. Die Auswertung zeigte außerdem, dass Okehampton ein sinnvolles „realistic worst-case“ Szenario für viele Substanzen darstellt. Wenn allerdings Substanzen nur eine geringe Sorption im Boden aufwiesen (Kfoc unterhalb von 30 L/kg), bilden andere Standorte den Worst Case besser ab (z.B. Hamburg oder Jokioinen). Piacenza (ein mediterranes Szenario) zeigte ebenfalls höhere Konzentrationen als Okehampton für diese Art von Substanzen. Deshalb wird vorgeschlagen, zusätzlich zu Okehampton auch Hamburg, Jokioinnen und Piacenza für die Grundwasserbewertung zu berücksichtigen.

Relevanz der FOCUS Standorte (Kompartiment Oberflächenwasser)

Im Gegensatz zu Grundwasser werden alle 10 Oberflächenwasserstandorte für die Risikoabschätzung von Tierarzneimitteln berücksichtigt. Da die Richtlinie für Futtermittelzusatzstoffe (EFSA 2007) nur einige FOCUS Szenarien empfiehlt, wurde auch für den Bereich Tierarzneimittel die Relevanz individueller Szenarien diskutiert. Um die Relevanz der Szenarien zu überprüfen wurden mit den neuesten Versionen von FOCUS SWASH (5.3), FOCUS MACRO (5.5.4), FOCUS PRZM (4.3.1) und FOCUS TOXSWA (5.5) Simulationen für 25 hypothetische Tierarzneimittel unter Berücksichtigung aller Szenarien durchgeführt. Parallele Simulationen wurden auch mit den Gleichungen der Stufe A (Tier A) gemacht. Die berechneten Konzentrationen zeigten folgende Abhängigkeit gegenüber Sorption und Abbau: Abnahme von Sorption und Abbau führten grundsätzlich zu einem Anstieg der Konzentration im Gewässer. Dies ist prinzipiell vergleichbar mit den Ergebnissen für Grundwasser. Es gibt allerdings einen wichtigen Unterschied im Vergleich zu Grundwasser: Angenommen, eine Substanz hat einen Kfoc von/oberhalb von 3000 L/kg, dann berechnet PEARL keinen Eintrag ins Grundwasser, sofern die DegT50 der jeweiligen Substanz nicht höher als 300 Tage ist. Dagegen können diese Substanzen über das Dränage System (D-Szenarien, durch präferentiellen Fluss) aber auch über Bodenerosion (R-Szenarien, durch Transport über die Sedimentphase) ins Gewässer gelangen.

Alternatives Mais-Szenario für Gülleapplikationen

Um den Einfluss eines alternativen Mais-Szenarios anstelle des Wintergetreide-Szenarios auf die Konzentration in Grund- und Oberflächenwasser zu untersuchen, wurden für eine Analyse die gleichen (hypothetischen) Tierarzneimittel wie in der vorherigen Auswertung ausgewählt. Auch das gleiche Applikationsmuster wurde verwendet (1 kg/ha 14 Tage vor dem Feldauflauf).

Bezogen auf Grundwasser wurde festgestellt, dass bei der Kultur Mais für kurzlebige Substanzen (Halbwertszeiten bis 30 Tage) signifikant niedrigere Konzentrationen berechnet werden als beim Wintergetreide. Hintergrund ist die unterschiedliche Jahreszeit bei der Applikation (Mais: Frühling, Wintergetreide: Herbst). Die dominante Zeit für die Versickerung stellt die Herbst/Winter-Periode dar. Bei einer Frühjahrsapplikation ist der Großteil der Substanz bereits abgebaut bevor der Herbst erreicht wurde. Allerdings war der Unterschied bei den Konzentrationen für Anwendungen in Mais oder Wintergetreide geringer, wenn die Substanzen persistenter waren (Halbwertszeit oberhalb von 100 Tagen). In einigen Fällen wurden sogar höhere Konzentrationen in Mais im Vergleich zu Wintergetreide berechnet (z.B. Substanzen mit einem Kfoc=100 L/kg am Standort Sevilla).

Ein ähnlicher Trend wurde auch für Oberflächenwasser gefunden: Die meisten Simulationen in Mais führten zu geringeren Konzentrationen als im Wintergetreide unabhängig von der Substanz. Allerdings gab es eine signifikante Ausnahme: Das R4-Bach-Szenario mit Mais führte grundsätzlich zu höheren Konzentrationen als mit Wintergetreide. Auch diese Situation wurde durch die unterschiedliche Anwendungszeit erklärt: Bei der R4-Wetterserie wird im Frühjahr eine ungünstigere Situation dargestellt als im Herbst. Diese Beobachtung könnte auch darauf hinweisen, dass ein einziges Simulationsjahr eine zu kurze Zeitperiode darstellt und sich die Situation nach Erweiterung der Simulationsperiode auf 20 Jahre mit der nächsten Aktualisierung des Modells ändert. Mais ist derzeit eine wichtige Kultur für die Ausbringung von Gülle. Deshalb wurde abschließend festgestellt, dass es sinnvoll wäre, auch Mais bei der Berechnung der Tierarzneimittelkonzentration in Grund- und Oberflächenwasser zu berücksichtigen.

Neues Szenario für Tierhaltung im Freiland

Derzeit gibt es keine Empfehlungen, wie die FOCUS Modelle eingesetzt werden können, wenn Tiere im Freiland auf der Weide gehalten werden. Dennoch könnten auch für diese Situation FOCUS Berechnungen erfolgen, vorausgesetzt einige Eingabeparameter werden angepasst. Vergleichbar der Berechnung bei der Intensivtierhaltung im Stall sollte die Anfangskonzentration im Boden die Basis für die Simulation darstellen. Die FOCUS Modelle verwenden einen täglichen Zeitschritt. Es wird deshalb empfohlen, die Applikationsrate (berechnet aus der Anfangskonzentration) über die Zeit einer Behandlung aufzuteilen. Wenn zum Beispiel die Tiere 5 Tage lang behandelt werden, sollte ein Fünftel der gesamten Applikationsmenge auf 5 aufeinanderfolgende Tage verteilt werden. Das würde zu einem realistischeren Applikationsmuster führen, als die Gesamtmenge an einem Tag auszubringen. Für die anderen Eingabeparameter wird empfohlen, die FOCUS-Kultur „grass/alfalfa“ mit festen Applikationsdaten (1. März oder 1 Oktober) zu verwenden. Applikationen sollten mit einer Einarbeitungstiefe von 0 cm simuliert werden. Ergebnisse mit den FOCUS Grundwasserszenarien für eine Substanz mit einem Kfoc von 300 L/kg und einer DegT50 von 100 Tagen führten zu deutlich niedrigen Konzentrationen als bei Wintergetreide und Mais, wenn 1 kg/ha auf 8 Tage verteilt wurden. Der allgemeine Trend bezogen auf die Rangfolge der Konzentrationen für die verschiedenen Standorte war allerdings ähnlich. Obwohl die Ergebnisse für andere Substanzen unterschiedlich sein könnten wurde festgestellt, dass die FOCUS Kultur „grass/alfalfa“ sinnvolle Ergebnisse liefert und für die Risikoabschätzung eingesetzt werden kann, wenn Tiere unter Freilandbedingungen gehalten werden.

Berücksichtigung von Risikominderungsmaßnahmen

Ursprünglich wurden bei den FOCUS Oberflächenwassermodellen drei Stufen ohne zusätzliche Verfeinerungen der Konzentrationen berücksichtigt (FOCUS 2001). Allerdings war es für die Risikoabschätzung bei Pestiziden erforderlich, eine zusätzliche Stufe einzubauen, in der Risikominderungsmaßnahmen berücksichtigt werden können. In diese Modellstufe wurden Verfeinerungen für Spraydrift (Pufferzonen, spezielle Düsen) und Runoff (bewachsene Pufferstreifen) berücksichtigt. Für die Dränage wurden keine Maßnahmen entwickelt. Für Tierarzneimittel wäre nur Runoff relevant, weil für alle Simulationen nur die Methode „Granulat“ verwendet wird, bei der keine Verdriftung simuliert wird.

Grundsätzlich könnte die Verfeinerung mit dem Programm SWAN erfolgen, wenn Standard FOCUS Simulationen vorliegen. Die Software unterstützt den Anwender bei der Modifizierung der vorliegenden Ergebnisdateien von PRZM (also der Runoff-Einträge) für diese spezielle Simulation. SWAN aktualisiert auch die TOXSWA Eingabedaten, so dass das Oberflächenwassermodell die veränderten PRZM Ergebnisdateien verwendet. Derzeit ist geplant, SWAN als offizielles Tool auf der FOCUS Internetseite zu etablieren.

Das EMA Dokument zu Risikominderung (EMA 2012) nennt minimale Abstände zum Oberflächengewässer als potentielle Maßnahme, wenn die Gülle von behandelten Tieren ausgebracht wird. Dies wäre methodisch identisch mit der finalen Stufe der FOCUS Oberflächenwasserszenarien. Deshalb wäre es technisch möglich, Konzentrationen im Gewässer zumindest für Standorte mit Puffersttriefen zu verfeinern. Allerdings wird in EMA (2012) diese Maßnahme als „nicht kontrollierbar für den Veterinär oder Landwirt“ klassifiziert und daher nicht empfohlen. Das bedeutet, dass die Maßnahme nicht EU-weit umgesetzt werden kann, obwohl es technisch für geeignete Standorte modelliert werden könnte.

Modellierung von ionisierenden Substanzen

Viele Tierarzneimittel sind ionisierend. Die Konsequenz ist, dass die Standardannahmen einer starken Korrelation von organischem Kohlenstoffgehalt im Boden und der Sorption nicht funktionieren. Richtlinien, wie diese Substanzen bewertet werden sollen, findet man in EMA (2018). Während bei der initialen Abschätzung (Tier A) der niedrigste Koc verwendet werden soll, soll für höherwertige Risikoabschätzungen der am besten geeignetste Adsorptionskoeffizient verwendet werden.

Der FOCUS GW Bericht (FOCUS 2009) gibt Empfehlungen, wie Substanzen, bei denen die Sorption vom pH-Wert im Boden abhängig ist, berechnet werden können. PEARL ist in der Lage, die pH-Wert-Abhängigkeit im Boden zu berechnen. Dabei wird angenommen, dass die Abhängigkeit durch unterschiedliche Anteile der ionisierten und der neutralen Form der Substanz in Abhängigkeit vom pH-Wert im Boden entsteht. Der Anwender muss die reinen Koc-Werte für beide Formen eintragen. Für die Abschätzung des jeweiligen Anteils in Abhängigkeit des pH ist zusätzlich der pKa der Substanz erforderlich. Der pKa Wert bestimmt bei welchem pH-Wert die Anteile beider Formen gleich groß sind.

Obwohl dieses Verfahren eine valide Transformation des Verhaltens von ionisierenden Substanzen darstellt, verletzt es dennoch die originale Definition der FOCUS Standorte als Worst-Case-Szenarien. Hintergrund ist, dass der Boden pH-Wert bei der Entwicklung der Szenarien nicht als Auswahlkriterium benutzt wurde. Deshalb ist anzunehmen, dass die pH-Werte der Standorte auch nicht Worst-Case-Bedingungen darstellen, so wie das für den Kohlenstoffgehalt im Boden oder das Klima der Fall ist. Daraus folgt, dass als einfache, praktikable und konservative Strategie auch eine Simulation auf Basis der Worst-Case-Sorptionskonstante im Labor (also des minimalen Werts) sinnvoll wäre. Die gleiche Worst-Case-Strategie könnte auch verfolgt werden, wenn die Sorptionskonstante mit anderen Bodenparameter korreliert (z.B. dem Tongehalt). Dies gilt auch für vom pH-Wert abhängige DegT50-Werte.

Der FOCUS SW Bericht (FOCUS 2001) diskutiert das Problem ionisierender Substanzen nicht. Unabhängig ob die Sorption mit dem Kohlenstoffgehalt im Boden korreliert oder ob Kfoc/DegT50-Werte vom pH-Wert abhängig sind, sollen mittlere Werte für die Simulation verwendet werden. Allerdings könnte es angemessener sein, für den Fall, dass die Parameter eindeutig pH-Wert abhängig sind, Worst-Case-Werte auszuwerten (also minimale Kfoc-Werte und maximale DegT50-Werte).

Handbuch

Am Ende des Berichtes befindet sich ein Handbuch zur Anwendung von FOCUS PEARL, FOCUS surface water und FOCUS SWAN für Tierarzneimittel.

1 Introduction

1.1 Initial situation

The use of veterinary compounds could have adverse effects on ecosystems in the environment. Therefore, before authorisation, an environmental risk assessment has to be conducted. An important part of the risk assessment for veterinary medicines is the evaluation of their exposure.

The risk assessment consists of several tiers. The initial calculation (Tier A assessment) follows straightforward equations using default values and information from the product literature. The refined calculation of groundwater concentrations for veterinary products is done based on the computer software FOCUS PEARL. Respective surface water simulations are performed using a software package with three different computer models (MACRO, PRZM, TOXSWA) connected by the shell SWASH.

Compared to the straightforward equations used for the Tier A assessment the Forum for international coordination of pesticide fate models and their use (FOCUS) developed higher tier numerical models with detailed environmental scenarios which describe realistic worst-case situations for major agricultural areas in Europe (FOCUS 2000). As surrogate for groundwater concentrations FOCUS uses percolate concentrations at a depth of 1 m. This assumption can be considered a conservative approach. With regard to surface water, FOCUS defined three entry routes (spray drift, run-off/erosion and drainage). Spray drift is not relevant for veterinary compounds since the substances are incorporated (no-drift situation). Run-off is overland flow occurring after heavy rainfall followed by the transport of substances into surface water via the solved phase. Together with run-off also suspended particles are transported into surface water bodies. Therefore, also substances with high sorption constants which do not appear in the water phase could be transported into surface water bodies via the sediment particles (soil erosion). The third entry route into surface water is transport via drainage system. Here only the water phase is considered (no particles in drainage water). FOCUS defined three different surface water bodies: ponds, ditches, and streams. Incoming water containing the substance due to run-off or drainage events is always diluted with water in the respective water system. Further dilution is caused by the upper water catchment area. Maximum concentrations are often relatively fast reduced by transport out of the system or by distribution to the sediment phase. That is shown in the models by additionally calculating time weighted average concentrations (TWA).

The idea of the groundwater scenarios was to combine the 80th spatial percentile (the soil scenarios) with the 80th temporal percentile (calculated based on a weather series of 20 years). That should result in an overall 90th percentile. Basically, also the FOCUS surface water scenarios aim at the overall 90th percentile for their simulations but the construction of the scenarios is less explicit. Especially the short simulation period of only a single year was often criticised which may have led to the formation of EFSA's FOCUS repair working group that recently recommended a simulation period of 20 years also for FOCUS surface water simulations (EFSA 2020). Unfortunately, the FOCUS SW models were not updated, yet at the time this report is written.

All models were developed and are provided by FOCUS for the risk assessment of plant protection products. Before the release of new versions of the models they are checked by an

EFSA guided working group (FOCUS version control). All models and manuals were originally developed for the registration of pesticides. However, this does not discredit the application of these models for veterinary compounds. The assumptions used in the model are valid also for other compounds as pesticides. It is just the forms of the existing shells which are not perfectly designed for the risk assessment of veterinary compounds. It is therefore consequent that FOCUS models are meanwhile used for the registration of all kinds of active substances (e.g., biocides, veterinary compounds). For veterinary compounds, the assessment is performed according to the guidance of VICH and the European Medicines Agency (EMA). Although the EMA guidance (as a supplement of the VICH guidance) contains some principles how input parameters should be considered and how results should be interpreted, especially for FOCUS SW simulations the recommendations are not specific enough. This complicates the use of the models for assessors and applicants and may sometimes lead to different model results.

1.2 Aim of the study

It was the aim of this project to suggest harmonised input parameters to be considered for the FOCUS groundwater model PEARL and the FOCUS Surface waters models (SWASH, PRZM, MACRO, TOXSWA) and to assess if the currently used options are still valid. Furthermore, instructions were developed about how the models should be used and how their results should be interpreted in the risk assessment. The results of this project were compiled in a way that it could serve as a base for development of a future manual for authorities and applicants when performing FOCUS simulations within the risk assessment. The study also investigated if FOCUS tools could be used to evaluate mitigation options for veterinary compounds.

Therefore, based on existing EMA guidance a manual was prepared about the use of the FOCUS models. In addition, this report contains suggestions about scientifically based improvements for the modelling. Furthermore, it points out possible technical problems or sources of error when using the models.

2 Recommendations for harmonised input parameter

2.1 Relevance of the FOCUS locations

2.1.1 Introduction

The FOCUS groundwater assessment is originally based on 9 different locations distributed over Europe. They are intended to represent major agricultural areas. However, currently only a single scenario (Okehampton) is used in the risk assessment for veterinary compounds. According to the current guideline "*... calculations by FOCUS [30] showed that the Hamburg, Okehampton and Piacenza scenarios gave the highest leaching concentrations of all scenarios for a few model substances (both for the PEARL, PRZM and PELMO models). The Hamburg scenario is considered not representative for areas with high intensity of livestock production. The Piacenza scenario is currently being reviewed by the FOCUS Groundwater Workgroup. It is likely that this scenario will be redefined by this workgroup because its representativeness is currently considered questionable. Thus, it seems most appropriate to base such a leaching assessment on the FOCUS Okehampton scenario. ...*" (EMA, 2005). However, meanwhile the Piacenza scenario was revised (FOCUS 2009/2014) and it will therefore be evaluated whether the original recommendations of 2005 should be updated and further scenarios should be considered for the risk assessment. It is furthermore important to notice that a FOCUS location like Hamburg was not just selected to represent the city but also for the agricultural area closed by with similar properties as Hamburg with regard to soil and climate conditions. As there are major agricultural areas with high intensity of livestock production south of Hamburg in Niedersachsen this location is considered suitable in contrast to EMA 2005.

In contrast to groundwater, all 10 surface water locations are considered relevant for the assessment of veterinary products. As the guidance for feed additives only recommends some scenarios for the respective target species (EFSA 2007), the relevance of individual scenarios has also been discussed for veterinary medicines.

Therefore, the relevance of the surface water scenarios will be also evaluated since it is expected that the next release of the FOCUS surface water scenarios will lead to a significant increase of the computer time for running the simulations (EFSA Repair action). Background is the change from a relatively short simulation period of 1 year to 20 years. That was necessary in order to improve modelling of surface water and drainage entries which are highly event based. Due to the short simulation period of only a single year the application could fall into a period without any run-off event or drain flow. In such a situation the risk assessment of surface water concentrations caused by these two processes was questionable.

It will therefore be checked which scenarios regularly show higher concentrations and should always be considered in the risk assessment. Consequently, scenarios could be omitted which normally show relatively low concentrations and because of that are of lower importance. It is also evaluated if certain scenarios are not relevant for veterinary medicines at all.

2.1.2 Relevance of the FOCUS groundwater scenarios

In order to check the relevance of the FOCUS groundwater scenarios simulations with the most recent version of FOCUS PEARL (which is 5.5.5) are performed for a variety of hypothetical veterinary compounds considering all FOCUS scenarios with input parameters:

- Kfoc (L/kg): 1, 3, 10, 30, 100, 300, 1000, 3000
- DegT50 (d): 1, 3, 10, 30, 100, 300

- Freundlich 1/n (-): 0.9
- Vapour pressure (Pa): 0
- Molecular mass (g/mol): 300
- Water solubility (mg/L): dependent on sorption: 100/Kfoc
- Application rate (kg/ha): 1 kg/ha
- Crops: winter cereals and maize
- Application date: 14 days before emergence
- Application depth (cm): 20
- Plant uptake factor (-) 0
- Locations: Winter cereals: all 9, maize: 8 (all except Jokioinen)

For all other substance specific input parameters, the default values were used. All combinations of 6 different DegT50 values and 8 different Kfoc values are considered for the simulations (48 variations). Applications of 1 kg/ha always 14 days before crop emergence are simulated for the two crops winter cereals and maize which finally results in 816 different calculations. In contrast to the supporting guidance relative application dates (14 days before emergence) were considered for the simulations. For Okehampton that will lead to an absolute application on October 3 which is exactly the recommended date. The advantage of using relative applications dates is that they guarantee for all locations always the same timing with regard to the crop development. This is important since crop development varies at the different FOCUS locations.

The results for the initial Tier A assessment is presented in Table 1.

Table 1: Results of PECgroundwater at Tier A, the initial risk assessment dependent on Koc (considering an application rate of 1 kg/ha related to 1333 µg/kg in 5 cm soil)

Koc (L/kg)	PECgw (µg/L)
1	2463.15
3	1953.53
10	1133.05
30	515.02
100	177.04
300	61.58
1000	18.76
3000	6.28

Results of the FOCUS PEARL simulations are presented for compounds with low, medium, and high sorption, respectively (Kfoc 1 L/kg (Table 2), Kfoc 100 L/kg (Table 3), and Kfoc 1000 L/kg (Table 4),. The chosen Koc values do not follow any formal classification of low/medium/high sorption, but simply serve to illustrate the impact of sorption on the FOCUS results. The results for all compounds considered in the evaluation are summarised in the appendix.

The FOCUS PEARL model always calculates concentrations below respective values determined using the equations of Tier A of the EMA GL.

Table 2: Results of FOCUS groundwater scenarios for compounds with very low sorption (Kfoc = 1 L/kg) when 1 kg/ha were incorporated 14 days before crop emergence of winter cereals (FOCUS PEARL 5.5.5, concentrations in µg/L)

DegT50 (d)	1	3	10	30	100	300
Châteaudun	0.001	0.605	20.715	111.228	386.992	707.023
Hamburg	0.172	14.959	110.398	315.554	530.003	621.420
Jokioinen	0.023	8.069	137.800	404.063	628.431	776.467
Kremsmünster	0.022	2.600	38.602	125.328	228.638	279.503
Okehampton	0.013	2.428	44.681	142.962	236.260	282.853
Piacenza	0.068	3.473	33.862	106.544	274.596	442.690
Porto	0.011	3.294	41.848	106.858	183.269	245.734
Sevilla	0.000	0.000	0.323	7.834	148.593	539.702
Thiva	0.001	0.615	13.801	77.261	408.502	1067.269

Table 3: Results of FOCUS groundwater scenarios for compounds with low sorption (Kfoc = 100 L/kg) when 1 kg/ha were incorporated 14 days before crop emergence of winter cereals (FOCUS PEARL 5.5.5, concentrations in µg/L)

DegT50 (d)	1	3	10	30	100	300
Châteaudun	0.000	0.000	0.000	0.488	35.730	191.060
Hamburg	0.000	0.000	0.034	4.734	63.954	205.423
Jokioinen	0.000	0.000	0.002	1.747	44.677	192.625
Kremsmünster	0.000	0.000	0.015	2.816	46.933	154.410
Okehampton	0.000	0.000	0.050	5.637	55.556	147.083
Piacenza	0.000	0.000	0.010	2.256	39.594	163.901
Porto	0.000	0.000	0.009	2.591	35.208	118.129
Sevilla	0.000	0.000	0.000	0.000	0.679	41.333
Thiva	0.000	0.000	0.000	0.117	31.253	300.893

Table 4: Results of FOCUS groundwater scenarios for compounds with high sorption (Kfoc = 1000 L/kg) when 1 kg/ha were incorporated 14 days before crop emergence of winter cereals (FOCUS PEARL 5.5.5, concentrations in µg/L)

DegT50 (d)	1	3	10	30	100	300
Châteaudun	0.000	0.000	0.000	0.000	0.000	0.034
Hamburg	0.000	0.000	0.000	0.000	0.003	2.199
Jokioinen	0.000	0.000	0.000	0.000	0.000	0.000
Kremsmünster	0.000	0.000	0.000	0.000	0.002	1.772
Okehampton	0.000	0.000	0.000	0.000	0.013	3.840
Piacenza	0.000	0.000	0.000	0.000	0.001	1.323
Porto	0.000	0.000	0.000	0.000	0.000	0.514
Sevilla	0.000	0.000	0.000	0.000	0.000	0.000
Thiva	0.000	0.000	0.000	0.000	0.000	0.000

With regard to the influence of sorption and degradation on the simulated concentrations, following (expected) results could be concluded: Decrease of sorption and of degradation always leads to an increase of the concentration in groundwater. Assuming the compound has a Kfoc of 3000 L/kg, the model does not simulate any concentrations for compounds with DegT50 up to 300 d (see the respective table in the appendix).

Aim of these simulations was to evaluate the relevance of alternative scenarios. In the following three tables the rank of the scenarios is presented with regard to their concentration in groundwater (1 means maximum concentration, 9 minimum concentration). The final column shows the average rank of the scenarios for a given sorption constant.

Table 5: Rank of FOCUS groundwater scenarios for compounds with low sorption (Kfoc = 1 L/kg) when 1 kg/ha were incorporated 14 days before crop emergence of winter cereals (FOCUS PEARL 5.5.5, concentrations in µg/L)

DegT50 (d)	1	3	10	30	100	300	Average
Châteaudun	8	8	7	5	4	3	7
Hamburg	1	1	2	2	2	4	2
Jokioinen	3	2	1	1	1	2	1
Kremsmünster	4	5	5	4	7	8	5
Okehampton	5	6	3	3	6	7	4
Piacenza	2	3	6	7	5	6	3
Porto	6	4	4	6	8	9	8
Sevilla	9	9	9	9	9	5	9
Thiva	7	7	8	8	3	1	6

Table 6: Rank of FOCUS groundwater scenarios for compounds with low sorption (Kfoc = 100 L/kg) when 1 kg/ha were incorporated 14 days before crop emergence of winter cereals (FOCUS PEARL 5.5.5, concentrations in µg/L)

DegT50 (d)	1	3	10	30	100	300	Average
Châteaudun	1	1	7	7	6	4	6
Hamburg	1	1	2	2	1	2	1
Jokioinen	1	1	6	6	4	3	4
Kremsmünster	1	1	3	3	3	6	3
Okehampton	1	1	1	1	2	7	2
Piacenza	1	1	4	5	5	5	4
Porto	1	1	5	4	7	8	6
Sevilla	1	1	8	9	9	9	9
Thiva	1	1	8	8	8	1	8

Table 7: Rank of FOCUS groundwater scenarios for compounds with high sorption (Kfoc = 1000 L/kg) when 1 kg/ha were incorporated 14 days before crop emergence of winter cereals (FOCUS PEARL 5.5.5, concentrations in µg/L)

DegT50 (d)	1	3	10	30	100	300	Average
Châteaudun	1	1	1	1	6	6	6
Hamburg	1	1	1	1	2	2	2
Jokioinen	1	1	1	1	6	7	7
Kremsmünster	1	1	1	1	3	3	3
Okehampton	1	1	1	1	1	1	1
Piacenza	1	1	1	1	4	4	4
Porto	1	1	1	1	5	5	5
Sevilla	1	1	1	1	6	9	9
Thiva	1	1	1	1	6	8	8

For low sorbing compounds (Kfoc = 1 L/kg) the results show Hamburg and Jokioinen are the worst-case locations, whereas for moderately (Kfoc = 100) and strongly sorbing compounds (Kfoc = 1000 L/kg) Hamburg and Okehampton showed maximum concentrations. However, these results do only consider a limited number of compounds. The final Table 8 shows the scenario ranking for all compounds considered in the study. The last column in this table shows that the previous results are confirmed even when looking at the maximum possible aggregation: Hamburg, Okehampton, and Jokioinen are the locations with in average highest concentrations in groundwater. All three locations represent moderate to cool temperature conditions. The worst-case scenario with Mediterranean conditions was found to be Piacenza (rank 4).

Table 8: Rank of FOCUS groundwater scenarios when comparing PECgw for compounds with DegT50s in the range of 1 d to 300 d when 1 kg/ha were incorporated 14 days before crop emergence of winter cereals

Kfoc (L/kg)	1	3	10	30	100	300	1000	3000	Average
Châteaudun	7	7	8	8	6	7	6	3	7
Hamburg	2	2	1	1	1	2	2	3	1
Jokioinen	1	1	2	2	4	6	7	3	3
Kremsmünster	5	4	3	7	3	3	3	3	5
Okehampton	4	5	5	3	2	1	1	2	2
Piacenza	3	3	3	4	4	4	4	1	4
Porto	8	7	7	4	6	5	5	3	6
Sevilla	9	9	9	9	9	9	9	3	9
Thiva	6	6	6	6	8	8	8	3	8

The evaluation showed that Okehampton represents a reasonable worst-case scenario for many compounds. However, the results also showed that for low sorbing compounds with Kfoc below 30 L/kg other scenarios (e.g., Hamburg, Jokioinen) are a better choice. Piacenza (as a Mediterranean location) also shows higher concentrations than Okehampton for this type of compounds. Therefore, in addition to Okehampton Hamburg, Jokioinen and Piacenza may be of relevance for the assessment of PECgw as well.

2.1.3 Relevance of the FOCUS surface water scenarios

In order to check the relevance of the FOCUS surface water simulations with the most recent versions of FOCUS SWASH (5.3), FOCUS MACRO (5.5.4), FOCUS PRZM (4.3.1) and FOCUS TOXSWA (5.5) were performed for a variety of hypothetical veterinary compounds considering all FOCUS scenarios with the following input parameters:

- DegT50 (d): 1, 3, 10, 30, 100, 300
- Kfoc (L/kg): 3, 30, 300, 3000
- Freundlich 1/n (-): 0.9
- Vapour pressure (Pa): 0
- Water solubility (mg/L): dependent on sorption: 100/Kfoc
- Molecular mass (g/mol): 300
- Application rate (kg/ha): 1 kg/ha
- Crops: winter cereals
- Application date: 14 days before emergence
- Application depth (cm): 20
- Plant uptake factor (-) 0

- Locations: D1 to D6, R1, R3, R4

For all other substance specific input parameters (e.g., molar enthalpies for vaporisation and dissolution), the default values in the model were used. These values represent defaults of the FOCUS guidance. All combinations of 6 different DegT50 values and 4 different Kfoc values are considered for the simulations (24 variations). Applications of 1 kg/ha are simulated always assuming the beginning of the application window at 14 days before crop emergence for winter cereals. This setting is also the default window in SWASH. These results finally in 144 PRZM simulations, 288 MACRO simulations and 672 different TOXSWA calculations. Based on these simulations it is decided which scenarios regularly show higher concentrations and should be always considered in the risk assessment. The results for the initial Tier A assessment is presented in Table 9.

Table 9: Results of PECsw at Tier A, the initial risk assessment dependent on Koc (considering an application rate of 1 kg/ha related to 1333 µg/kg in 5 cm soil)

Koc (L/kg)	PECsw (µg/L)
1	821.05
3	651.18
10	377.68
30	171.67
100	59.01
300	20.53
1000	6.25
3000	2.09

All FOCUS results are presented in the following tables with concentrations in surface water for compounds with Kfoc 3 L/kg (Table 10), Kfoc 30 L/kg (Table 11), Kfoc 300 L/kg (Table 12), and Kfoc 3000 L/kg (Table 13), respectively. In most situations the FOCUS models calculate concentrations below respective values of Tier A. However, the scenario D2 is sometimes an exception. D2 is an extreme worst-case with regard to its soil properties (heavy soil with more than 50% clay, see FOCUS 2001). This is a problematic situation for the tiered risk assessment. Obviously, the assumed dilution factor at Tier A (factor 3) is higher than the dilution simulated for this FOCUS scenario. The situation may hopefully change when the updated FOCUS models with their increased simulation period become available. If the situation does not change it may have to be considered to increase the conservativeness of the initial risk assessment (e.g., dilution factor of only 2 instead of 3).

Table 10: Results of FOCUS surface water scenarios for compounds with very low sorption (Kfoc = 3 L/kg) when 1 kg/ha were incorporated (FOCUS TOXSWA 5.5, Begin of application window: 14 days before crop emergence of winter cereals, concentrations in µg/L)

DegT50 (d)	1	3	10	30	100	300
D1_Ditch	0.832	7.924	28.870	51.550	70.610	104.600
D1_Stream	0.627	5.764	19.640	33.940	45.580	65.650
D2_Ditch	20.540	79.400	127.700	147.600	162.500	176.500
D2_Stream	13.590	51.890	83.090	95.870	105.400	114.200
D3_Ditch	0.008	1.728	21.950	56.250	89.510	106.500
D4_Pond	0.000	0.066	8.779	50.290	134.700	197.100
D4_Stream	0.001	0.164	7.547	34.710	69.910	89.840
D5_Pond	0.007	1.897	23.050	56.720	124.500	210.000
D5_Stream	0.049	2.327	17.020	34.920	60.720	84.230
D6_Ditch	1.130	9.290	20.260	27.520	43.050	83.390
R1_Pond	0.013	0.028	0.036	0.039	0.040	0.040
R1_Stream	1.253	2.595	3.345	3.595	3.689	3.715
R3_Stream	2.860	6.594	8.814	9.586	9.861	9.942
R4_Stream	0.000	0.003	0.017	0.030	0.036	0.038

Table 11: Results of FOCUS surface scenarios for compounds with low sorption (Kfoc = 30 L/kg) when 1 kg/ha were incorporated (FOCUS TOXSWA 5.5, Begin of application window: 14 days before crop emergence of winter cereals, concentrations in µg/L)

DegT50 (d)	1	3	10	30	100	300
D1_Ditch	0.692	9.672	36.070	62.800	84.130	97.670
D1_Stream	0.513	6.849	24.380	41.290	54.390	62.870
D2_Ditch	21.090	85.250	139.000	161.200	177.800	192.400
D2_Stream	13.370	53.760	87.360	101.200	111.600	120.800
D3_Ditch	0.000	0.002	0.377	4.939	32.020	68.550
D4_Pond	0.000	0.021	2.240	15.180	70.240	142.100
D4_Stream	0.001	0.032	3.026	13.590	34.150	62.150
D5_Pond	0.004	0.385	5.555	13.600	41.310	120.200
D5_Stream	0.036	1.756	7.030	10.990	21.320	47.730
D6_Ditch	1.463	11.580	24.510	31.510	39.080	59.750
R1_Pond	0.017	0.037	0.048	0.052	0.054	0.054

DegT50 (d)	1	3	10	30	100	300
R1_Stream	1.584	3.442	4.511	4.874	5.007	5.046
R3_Stream	2.472	5.859	7.915	8.625	8.887	8.962
R4_Stream	0.000	0.017	0.106	0.177	0.213	0.224

Table 12: Results of FOCUS surface scenarios for compounds with moderate sorption (Kfoc = 300 L/kg) when 1 kg/ha were incorporated (FOCUS TOXSWA 5.5, Begin of application window: 14 days before crop emergence of winter cereals, concentrations in µg/L)

DegT50 (d)	1	3	10	30	100	300
D1_Ditch	0.001	1.335	13.940	44.190	74.080	93.930
D1_Stream	0.001	0.984	9.311	27.670	46.320	58.700
D2_Ditch	0.003	4.742	43.410	80.520	106.400	123.100
D2_Stream	0.002	3.018	27.130	50.130	66.240	76.700
D3_Ditch	0.000	0.000	0.000	0.000	0.000	0.077
D4_Pond	0.000	0.004	1.157	5.197	11.340	19.840
D4_Stream	0.000	0.012	1.451	6.067	12.770	20.610
D5_Pond	0.000	0.178	3.119	7.050	11.990	20.620
D5_Stream	0.000	0.301	4.099	8.557	13.010	18.500
D6_Ditch	0.146	6.387	20.900	29.320	34.780	42.080
R1_Pond	0.007	0.019	0.045	0.058	0.064	0.066
R1_Stream	0.641	1.567	2.141	2.339	2.413	2.435
R3_Stream	0.766	2.001	2.797	3.075	3.177	3.207
R4_Stream	0.000	0.092	0.802	1.479	1.831	1.946

Table 13: Results of FOCUS surface scenarios for compounds with high sorption (Kfoc = 3000 L/kg) when 1 kg/ha were incorporated (FOCUS TOXSWA 5.5, Begin of application window: 14 days before crop emergence of winter cereals, concentrations in µg/L)

DegT50 (d)	1	3	10	30	100	300
D1_Ditch	0.000	0.000	0.000	0.001	1.808	10.730
D1_Stream	0.000	0.000	0.000	0.001	1.137	6.733
D2_Ditch	0.000	0.000	0.000	0.072	6.889	15.960
D2_Stream	0.000	0.000	0.000	0.047	5.863	9.998
D3_Ditch	0.000	0.000	0.000	0.000	0.000	0.000
D4_Pond	0.000	0.000	0.002	0.014	0.147	0.681

DegT50 (d)	1	3	10	30	100	300
D4_Stream	0.000	0.000	0.021	0.124	0.737	2.510
D5_Pond	0.000	0.000	0.003	0.007	0.025	0.243
D5_Stream	0.000	0.003	0.043	0.105	0.255	1.033
D6_Ditch	0.000	0.014	0.502	1.390	3.121	9.856
R1_Pond	0.001	0.011	0.028	0.037	0.047	0.056
R1_Stream	0.066	0.166	0.230	0.257	0.306	0.356
R3_Stream	0.076	0.208	0.294	0.325	0.352	0.421
R4_Stream	0.000	0.017	0.176	0.344	0.449	0.504

With regard to the influence of sorption and degradation on the simulated concentrations, following (expected) results could be concluded: Decrease of sorption and of degradation always lead to an increase of the concentration in surface water. This is principally comparable to the results of the FOCUS groundwater scenarios. There is, however, an important difference to groundwater. Assuming the compound has a Kfoc of 3000 L/kg, PEARL does not simulate any concentrations for compounds with DegT50 up to 300 d in groundwater (see the respective table in the appendix). In contrast, these compounds could be transported into surface water through the drainage system (see the results for D-scenarios in Table 13), but also due to soil erosion (see the results for R-scenarios in the same Table 13).

The following Table 14 shows the selection of scenarios for feed additives according to the EFSA guideline EFSA (2007).

Table 14: Proposed FOCUS SW scenarios for PEC surface water calculation for feed additives (Table 7 of EFSA (2007)

	FOCUS SW (Drainage)	Consideration
Bovine	D4	Highly significant northern European livestock production scenario (major livestock production region).
Ovine	D6	Highly significant Mediterranean/Southern European livestock production scenarios (major livestock production regions).
Swine	D4, D3	Highly significant northern European livestock production scenarios (major livestock production regions).
Avian	D5, D3	Highly significant northern European livestock production scenarios (major livestock production regions).
	FOCUS SW (runoff)	**Consideration**
Bovine	R3, R1	Runoff scenario of greatest regional, pedoclimatic relevance to livestock production.
Ovine	R4	Runoff scenario of greatest regional, pedoclimatic relevance to livestock production. Ovine production associated with R4 pedoclimatic conditions is comparatively minor.
Swine	R3, R1	Runoff scenario of greatest regional, pedoclimatic relevance to livestock production.
Avian	R3, R1	Runoff scenario of greatest regional, pedoclimatic relevance to livestock production.

Depending on the target animal only a small number of locations are considered. According to a recent study by (Haupt et al. 2021) the strict categorisation of animals to locations is not defensible. There are more variations of animal keeping especially as the FOCUS locations represent not just a spot but a major agricultural region in Europe. In addition, it is common practice to transport manure between regions (Garbs and Geldermann 2018, Kuhn et al. 2018).

Beyond that in this evaluation the relevance of scenarios is purely analysed with regard to their results (similar to the analysis of the groundwater location in the previous section). Consequently, in the following tables 1 means maximum concentration (absolute worst-case) whereas 14 means minimum concentration. The final column always shows the average rank of the scenarios for a given sorption constant.

Table 15: Rank of FOCUS surface water scenarios for compounds with very low sorption (Kfoc = 3 L/kg) when 1 kg/ha were incorporated 14 days before crop emergence of winter cereals (FOCUS TOXSWA 5.5, concentrations in µg/L)

DegT50 (d)	1	3	10	30	100	300	Average
D1_Ditch	6	4	3	5	6	6	3
D1_Stream	7	6	7	9	9	10	9
D2_Ditch	1	1	1	1	1	3	1
D2_Stream	2	2	2	2	4	4	2
D3_Ditch	10	10	5	4	5	5	5
D4_Pond	13	12	10	6	2	2	7
D4_Stream	12	11	11	8	7	7	11
D5_Pond	11	9	4	3	3	1	4
D5_Stream	8	8	8	7	8	8	8
D6_Ditch	5	3	6	10	10	9	6
R1_Pond	9	13	13	13	13	13	13
R1_Stream	4	7	12	12	12	12	12
R3_Stream	3	5	9	11	11	11	10
R4_Stream	14	14	14	14	14	14	14

Table 16: Rank of FOCUS surface water scenarios for compounds with low sorption (Kfoc = 30 L/kg) when 1 kg/ha were incorporated 14 days before crop emergence of winter cereals (FOCUS TOXSWA 5.5, concentrations in µg/L)

DegT50 (d)	1	3	10	30	100	300	Average
D1_Ditch	6	4	3	3	3	5	3
D1_Stream	7	5	5	4	5	7	4
D2_Ditch	1	1	1	1	1	1	1
D2_Stream	2	2	2	2	2	3	2
D3_Ditch	14	14	12	11	9	6	12

DegT50 (d)	1	3	10	30	100	300	Average
D4_Pond	12	12	11	6	4	2	7
D4_Stream	11	11	10	8	8	8	10
D5_Pond	10	9	8	7	6	4	6
D5_Stream	8	8	7	9	10	10	9
D6_Ditch	5	3	4	5	7	9	4
R1_Pond	9	10	14	14	14	14	13
R1_Stream	4	7	9	12	12	12	10
R3_Stream	3	6	6	10	11	11	7
R4_Stream	13	13	13	13	13	13	14

Table 17: Rank of FOCUS surface water scenarios for compounds with moderate sorption (Kfoc = 300 L/kg) when 1 kg/ha were incorporated 14 days before crop emergence of winter cereals (FOCUS TOXSWA 5.5, concentrations in µg/L)

DegT50 (d)	1	3	10	30	100	300	Average
D1_Ditch	7	6	4	3	2	2	4
D1_Stream	8	7	5	5	4	4	5
D2_Ditch	5	2	1	1	1	1	1
D2_Stream	6	3	2	2	3	3	2
D3_Ditch	12	14	14	14	14	13	14
D4_Pond	12	13	11	9	9	8	11
D4_Stream	12	12	10	8	7	7	10
D5_Pond	11	9	7	7	8	6	8
D5_Stream	9	8	6	6	6	9	7
D6_Ditch	3	1	3	4	5	5	3
R1_Pond	4	11	13	13	13	14	13
R1_Stream	2	5	9	11	11	11	9
R3_Stream	1	4	8	10	10	10	6
R4_Stream	9	10	12	12	12	12	12

Table 18: Rank of FOCUS surface water scenarios for compounds with high sorption (Kfoc = 3000 L/kg) when 1 kg/ha were incorporated 14 days before crop emergence of winter cereals (FOCUS TOXSWA 5.5, concentrations in µg/L)

DegT50 (d)	1	3	10	30	100	300	Average
D1_Ditch	6	10	12	12	4	2	9
D1_Stream	6	10	12	13	5	5	11
D2_Ditch	6	10	10	7	1	1	5
D2_Stream	6	10	10	8	2	3	7
D3_Ditch	6	10	12	14	14	14	14
D4_Pond	6	9	9	10	11	8	12
D4_Stream	6	8	7	5	6	6	6
D5_Pond	6	7	8	11	13	12	13
D5_Stream	5	6	5	6	10	7	7
D6_Ditch	6	4	1	1	3	4	1
R1_Pond	3	5	6	9	12	13	10
R1_Stream	2	2	3	4	9	11	4
R3_Stream	1	1	2	3	8	10	2
R4_Stream	4	3	4	2	7	9	3

The pattern of results very much depends on the interaction of compound properties and scenario type:

- For low and moderately sorbing compounds (i.e., Kfoc = 3 L/kg up to 300 L/kg, see Table 15 to Table 17) D2, ditch and stream, represent the worst-case situation followed by the other drainage scenarios. This is not very much dependent on the half-life of the compound. For these compounds the R1 pond and the R4 stream generally leads to the lowest concentrations. Low sorbing compounds with slow degradation are calculated with higher concentrations in D4/D5 ponds than in D4/D5 streams. Background is the little outflow in ponds compared to streams which may lead to some accumulation.
- If compounds sorb strongly to soil (Kfoc = 3000 L/kg, see Table 18) still D2 (ditch and stream) represent maximum concentrations in case the compound is only slowly degrading (DegT50 in soil above 100 days). If, however, the respective substance degrades fast the run-off stream scenarios represent worst-case conditions (R1 and R3). Minimum concentrations are calculated for all drainage scenarios especially D3 when a strongly sorbing compound degrades fast (i.e. DegT50 below 100 days).

The final Table 19 shows the results of the previous four tables in maximum possible aggregation: considering the spectrum of artificial substances, the D-stream scenarios, except D3, usually represent worst-case situations. D3 (Vredepeel in the Netherlands with its sandy soil) is different because in this scenario macro-pore flow is not considered. The run-off scenarios are dominant if the sorption constant is high (see Kfoc = 3000 L/kg in Table 19) because they also consider particle-bound transport due to erosion. For pond scenarios, especially R1 pond minimum concentrations are calculated independent of sorption and degradation properties of the compound. Background is especially the depth and width of the ponds (high water volume) which leads to more dilution compared to streams and ditches.

Table 19: Rank of FOCUS surface water scenarios when comparing PECsw for compounds with DegT50s in the range of 1 d to 300 d when 1 kg/ha were incorporated 14 days before crop emergence of winter cereals

Kfoc (L/kg)	3	30	300	3000	Average
D1_Ditch	3	3	4	9	4
D1_Stream	9	4	5	11	6
D2_Ditch	1	1	1	5	1
D2_Stream	2	2	2	7	2
D3_Ditch	5	12	14	14	13
D4_Pond	7	7	11	12	10
D4_Stream	11	10	10	6	10
D5_Pond	4	6	8	13	7
D5_Stream	8	9	7	7	7
D6_Ditch	6	4	3	1	3
R1_Pond	13	13	13	10	14
R1_Stream	12	10	9	4	9
R3_Stream	10	7	6	2	5
R4_Stream	14	14	12	3	12

2.2 Application scenarios for veterinary compounds

2.2.1 Introduction

For the risk assessment of veterinary compounds only a single application scenario (manure application to winter cereals in autumn before crop emergence) is currently considered. In order to assess the relevance of alternative scenarios, manure applications in maize are simulated since maize is of increasing importance in European agriculture and a representative example for a spring crop. Compared to winter cereals, the pre-emergence application in maize would be performed at a very different season.

Furthermore, there is presently no advice given on the calculation of exposure via runoff and drainage for pasture animals. The supporting GL describes the scenario for direct entry which usually leads to higher results than runoff scenarios on arable land for the same product. However, for those cases where emission into water from direct entry can be mitigated, the exposure pathway runoff still needs to be considered for application of manure to arable land as well as for pasture animals. There was some uncertainty whether it is correct to apply the FOCUS surface water models also for pasture scenarios.

2.2.2 Alternative maize scenario for manure applications

2.2.2.1 Entry route groundwater (FOCUS PEARL)

In order to check the impact of using the alternative maize scenario instead of winter cereals the same compounds were used as in the previous section 2.1.2 (48 combinations of compounds with Kfoc in the range of 1 L/kg to 3000 L/kg and DegT50 in the range of 1 d to 300 d). Also, the application pattern did not change (1 kg/ha 14 days before crop emergence).

For an optimum comparison results are presented in the same way as in section 2.1.2, so Table 20 shows results for compounds with Kfoc = 1 L/kg, Table 21 for compounds with Kfoc = 100 L/kg, and Table 22 for compounds with Kfoc = 1000 L/kg, respectively. The results for all compounds considered in the evaluation are again summarised in the appendix. FOCUS did not define a maize scenario for Jokioinen (probably because of the cold weather conditions). All other locations are represented.

Table 20: Results of FOCUS groundwater scenarios for compounds with low sorption (Kfoc = 1 L/kg) when 1 kg/ha were incorporated 14 days before crop emergence of winter cereals (FOCUS PEARL 5.5.5, concentrations in µg/L)

DegT50 (d)	1	3	10	30	100	300
Châteaudun	0.000	0.000	1.550	53.686	236.160	377.637
Hamburg	0.000	0.008	7.115	108.469	344.694	490.832
Kremsmünster	0.000	0.034	5.511	65.419	193.984	277.346
Okehampton	0.000	0.038	6.123	61.775	173.108	250.909
Piacenza	0.000	0.005	1.648	33.582	210.140	390.657
Porto	0.000	0.002	0.723	20.850	105.714	161.508
Sevilla	0.000	0.000	0.011	4.593	117.058	436.181
Thiva	0.000	0.000	0.112	24.941	298.387	682.978

Table 21: Results of FOCUS groundwater scenarios for compounds with low sorption (Kfoc = 100 L/kg) when 1 kg/ha were incorporated 14 days before crop emergence of winter cereals (FOCUS PEARL 5.5.5, concentrations in µg/L)

DegT50 (d)	1	3	10	30	100	300
Châteaudun	0.000	0.000	0.000	0.434	33.489	161.730
Hamburg	0.000	0.000	0.001	1.403	47.488	191.324
Kremsmünster	0.000	0.000	0.001	1.211	36.369	142.820
Okehampton	0.000	0.000	0.004	2.241	43.380	128.467
Piacenza	0.000	0.000	0.001	0.959	32.090	167.417
Porto	0.000	0.000	0.000	0.206	17.116	77.273
Sevilla	0.000	0.000	0.000	0.003	5.720	103.761
Thiva	0.000	0.000	0.000	0.056	27.000	244.360

Table 22: Results of FOCUS groundwater scenarios for compounds with high sorption (Kfoc = 1000 L/kg) when 1 kg/ha were incorporated 14 days before crop emergence of winter cereals (FOCUS PEARL 5.5.5, concentrations in µg/L)

DegT50 (d)	1	3	10	30	100	300
Châteaudun	0.000	0.000	0.000	0.000	0.000	0.425
Hamburg	0.000	0.000	0.000	0.000	0.002	1.844
Kremsmünster	0.000	0.000	0.000	0.000	0.001	1.529
Okehampton	0.000	0.000	0.000	0.000	0.008	3.487
Piacenza	0.000	0.000	0.000	0.000	0.001	1.832
Porto	0.000	0.000	0.000	0.000	0.000	0.399
Sevilla	0.000	0.000	0.000	0.000	0.000	0.000
Thiva	0.000	0.000	0.000	0.000	0.000	0.067

Similar as for winter cereals the influence of sorption and degradation on the simulated concentrations follows the (expected) results: Decrease of sorption and of degradation always leads to an increase of the concentration in groundwater. Assuming the compound has a Kfoc of 3000 L/kg the model does not simulate any concentrations for compounds with DegT50 up to 300 d (see the respective table in appendix A).

Aim of these simulations was to compare the two crops with regard to their calculated concentrations in groundwater. The difference is calculated according to following equation:

$$Diff = \frac{C_{MZ} - C_{WC}}{C_{WC}} \cdot 100$$

C_{MZ} Concentration for maize (µg/L)

C_{WC} Concentration for winter cereals (µg/L)

Diff Difference between result for maize and winter cereals (%)

In the following Table 23 to Table 25 the differences of the maize scenario to the respective winter scenario is presented for compounds with three different sorption constants Kfoc.

Table 23: Relative difference (%) of concentrations for applications to maize instead of winter cereals.

Results of FOCUS groundwater scenarios for compounds with low sorption (Kfoc = 1 L/kg) when 1 kg/ha were incorporated 14 days before crop emergence (FOCUS PEARL 5.5.5)

DegT50 (d)	1	3	10	30	100	300
Châteaudun	n.a.	-99.9	-92.5	-51.7	-39.0	-46.6
Hamburg	-100.0	-99.9	-93.6	-65.6	-35.0	-21.0
Kremsmünster	-99.8	-98.7	-85.7	-47.8	-15.2	-0.8

DegT50 (d)	1	3	10	30	100	300
Okehampton	-98.6	-98.4	-86.3	-56.8	-26.7	-11.3
Piacenza	-100.0	-99.9	-95.1	-68.5	-23.5	-11.8
Porto	-100.0	-100.0	-98.3	-80.5	-42.3	-34.3
Sevilla	n.a.	n.a.	-96.7	-41.4	-21.2	-19.2
Thiva	n.a.	-100.0	-99.2	-67.7	-27.0	-36.0

n.a. not applicable because the results of FOCUS PEARL for winter cereals was below 0.001 µg/L

Table 24: Relative difference (%) of concentrations for applications to maize instead of winter cereals.

Results of FOCUS groundwater scenarios for compounds with low sorption (Kfoc = 100 L/kg) when 1 kg/ha were incorporated 14 days before crop emergence (FOCUS PEARL 5.5.5)

DegT50 (d)	1	3	10	30	100	300
Châteaudun	n.a.	n.a.	n.a.	-11.2	-6.3	-15.4
Hamburg	n.a.	n.a.	-98.2	-70.4	-25.7	-6.9
Kremsmünster	n.a.	n.a.	-95.5	-57.0	-22.5	-7.5
Okehampton	n.a.	n.a.	-92.6	-60.3	-21.9	-12.7
Piacenza	n.a.	n.a.	-93.5	-57.5	-19.0	2.1
Porto	n.a.	n.a.	-100.0	-92.0	-51.4	-34.6
Sevilla	n.a.	n.a.	n.a.	n.a.	742.9	151.0
Thiva	n.a.	n.a.	n.a.	-52.3	-13.6	-18.8

n.a. not applicable because the results of FOCUS PEARL for winter cereals was below 0.001 µg/L

Table 25: Relative difference (%) of concentrations for applications to maize instead of winter cereals.

Results of FOCUS groundwater scenarios for compounds with strong sorption (Kfoc = 1000 L/kg) when 1 kg/ha were incorporated 14 days before crop emergence (FOCUS PEARL 5.5.5)

DegT50 (d)	1	3	10	30	100	300
Châteaudun	n.a.	n.a.	n.a.	n.a.	n.a.	1168.2
Hamburg	n.a.	n.a.	n.a.	n.a.	-35.5	-16.2
Kremsmünster	n.a.	n.a.	n.a.	n.a.	-36.8	-13.7
Okehampton	n.a.	n.a.	n.a.	n.a.	-33.4	-9.2
Piacenza	n.a.	n.a.	n.a.	n.a.	n.a.	38.5
Porto	n.a.	n.a.	n.a.	n.a.	n.a.	-22.3
Sevilla	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
Thiva	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.

n.a. not applicable because the results of FOCUS PEARL for winter cereals was below 0.001 µg/L

Most of the differences shown in Table 23 to Table 25 are negative which means for maize lower concentrations were simulated than for winter cereals. No comparison was made if the concentrations in winter cereals were below 0.001 µg/L. The minimum value in the table (i.e., -100 %) means concentration of 0 for maize and concentrations above 0.001 µg/L in winter cereals. The general trend is that significantly lower concentrations were simulated in maize than in winter cereals for short living compounds (half lives up to 30 days). Background is the different application season (spring in maize, autumn in winter cereals). The dominant season for leaching is in autumn/winter period. Most of the applied compounds are already degraded before autumn is reached when they are applied in spring. If, however, the compounds are more persistent (half-life above 100 days) the difference between autumn and spring application becomes less relevant and occasionally even higher concentrations are simulated in maize than in winter cereals (e.g., compounds with Kfoc = 100 L/kg at Sevilla, see Table 21).

It can be concluded that the results of the alternative maize scenario are in line with expert judgement: short living compounds applied in spring are simulated with significantly lower concentrations. As maize is currently an important crop for the application of manure it would make sense to also consider maize in the risk assessment for veterinary compounds when assessing the leaching of these substances to groundwater.

2.2.2.2 Entry route surface water (FOCUS TOXSWA 5.5)

In order to check the impact of using the alternative maize scenario instead of winter cereals the same compounds are considered as in the previous section 2.1.3 (24 combinations of compounds with Kfoc in the range of 3 L/kg to 3000 L/kg and DegT50 in the range of 1 d to 300 d). Also, the application pattern did not change (1 kg/ha 14 days before crop emergence).

All results are presented in the following tables with concentrations in surface water for compounds with Kfoc = 3 L/kg (Table 26), Kfoc = 30 L/kg (Table 27), Kfoc = 300 L/kg (Table 28), and Kfoc = 3000 L/kg (Table 29), respectively. FOCUS did not define a maize scenario (but a winter cereal scenario) for the location D1 (Lanna, Sweden) and D2 (Brimsone, UK), probably because of the cold weather conditions. In contrast FOCUS did not define a scenario for winter cereals but a maize scenario at R2 (Porto). This was as also because of climatic reasons.

Table 26: Results of FOCUS surface water scenarios for compounds with very low sorption (Kfoc = 3 L/kg) when 1 kg/ha were incorporated (FOCUS TOXSWA 5.5, Begin of application window: 14 days before crop emergence of maize, concentrations in µg/L)

DegT50 (d)	1	3	10	30	100	300
D3_Ditch	0.000	0.001	0.893	14.620	51.300	78.730
D4_Pond	0.000	0.001	0.307	11.230	77.400	147.100
D4_Stream	0.000	0.002	4.431	6.809	37.050	65.790
D5_Pond	0.000	0.000	0.226	5.405	58.470	150.900
D5_Stream	0.000	0.000	4.687	3.514	30.580	77.450
D6_Ditch	0.008	0.058	0.179	1.252	14.930	56.830
R1_Pond	0.001	0.003	0.006	0.007	0.008	0.008

DegT50 (d)	1	3	10	30	100	300
R1_Stream	0.098	0.617	1.163	1.391	1.482	1.509
R2_Stream	0.005	0.168	0.554	0.777	0.875	0.906
R3_Stream	0.000	0.001	0.003	0.005	0.006	0.006
R4_Stream	0.377	2.431	4.663	5.617	5.995	6.107

Table 27: Results of FOCUS surface water scenarios for compounds with low sorption (Kfoc = 30 L/kg) when 1 kg/ha were incorporated (FOCUS TOXSWA 5.5, Begin of application window: 14 days before crop emergence of maize, concentrations in µg/L)

DegT50 (d)	1	3	10	30	100	300
D3_Ditch	0.000	0.000	0.001	1.546	23.950	59.640
D4_Pond	0.000	0.000	0.013	3.100	43.880	117.000
D4_Stream	0.000	0.000	0.012	2.224	21.970	50.060
D5_Pond	0.000	0.000	0.014	1.105	21.960	102.600
D5_Stream	0.000	0.000	0.018	0.785	10.870	41.970
D6_Ditch	0.004	0.038	0.136	0.509	7.078	32.910
R1_Pond	0.001	0.004	0.009	0.011	0.013	0.014
R1_Stream	0.114	0.841	1.671	2.030	2.173	2.215
R2_Stream	0.007	0.369	1.389	2.017	2.297	2.384
R3_Stream	0.000	0.005	0.034	0.057	0.069	0.073
R4_Stream	0.340	2.275	4.406	5.318	5.681	5.789

Table 28: Results of FOCUS surface water scenarios for compounds with moderate sorption (Kfoc = 300 L/kg) when 1 kg/ha were incorporated (FOCUS TOXSWA 5.5, Begin of application window: 14 days before crop emergence of maize, concentrations in µg/L)

DegT50 (d)	1	3	10	30	100	300
D3_Ditch	0.000	0.000	0.000	0.000	0.001	0.260
D4_Pond	0.000	0.000	0.002	0.529	4.469	12.750
D4_Stream	0.000	0.000	0.003	0.597	4.925	12.790
D5_Pond	0.000	0.000	0.212	0.202	2.987	10.240
D5_Stream	0.000	0.000	4.673	0.236	2.694	8.074
D6_Ditch	0.000	0.000	0.001	0.200	2.445	9.101
R1_Pond	0.000	0.006	0.034	0.066	0.082	0.689
R1_Stream	0.038	0.394	0.889	1.120	1.215	12.040

DegT50 (d)	1	3	10	30	100	300
R2_Stream	0.001	0.100	0.464	0.718	0.837	8.820
R3_Stream	0.000	0.019	0.335	0.744	0.980	8.392
R4_Stream	0.148	1.228	2.543	3.127	3.361	32.200

Table 29: Results of FOCUS surface water scenarios for compounds with high sorption (Kfoc = 3000 L/kg) when 1 kg/ha were incorporated (FOCUS TOXSWA 5.5, Begin of application window: 14 days before crop emergence of maize, concentrations in µg/L)

DegT50 (d)	1	3	10	30	100	300
D3_Ditch	0.000	0.000	0.000	0.000	0.000	0.000
D4_Pond	0.211	0.000	0.000	0.003	0.081	0.558
D4_Stream	4.306	0.000	0.000	0.023	0.424	4.306
D5_Pond	0.000	0.000	0.000	0.000	0.011	0.132
D5_Stream	0.000	0.000	0.000	0.005	0.116	0.641
D6_Ditch	0.000	0.000	0.000	0.005	0.715	4.325
R1_Pond	0.000	0.001	0.009	0.020	0.039	0.081
R1_Stream	0.004	0.042	0.124	0.209	0.291	0.358
R2_Stream	0.000	0.009	0.043	0.068	0.090	0.121
R3_Stream	0.000	0.003	0.075	0.186	0.268	0.332
R4_Stream	0.017	0.170	0.376	0.472	0.525	0.561

Similar as for winter cereals, the influence of sorption and degradation on the simulated concentrations follows the (expected) results: Decrease of sorption and degradation always leads to an increase of the concentration in groundwater. In line with FOCUS SW simulations in winter cereals concentrations in surface water are also simulated when the compound strongly sorbs to soil (see Table 29). The same conclusions can be drawn for maize as for winter cereals: Strongly sorbing compounds could be transported into surface water through the drainage system (i.e., results for D-scenarios in Table 29), but also due to soil erosion (i.e., results for R-scenarios in the same Table 29).

Aim of these simulations was to compare the two crops with regard to their calculated concentrations in groundwater. The difference is calculated according to the equation presented in section 2.2.2.1.

Table 30: Relative difference (%) of concentrations for applications to maize instead of winter cereals.

Results of FOCUS surface water scenarios for compounds with low sorption (Kfoc = 3 L/kg) when 1 kg/ha were incorporated 14 days before crop emergence (FOCUS TOXSWA 5.5)

DegT50 (d)	1	3	10	30	100	300
D3_Ditch	-100.0	-99.9	-95.9	-74.0	-42.7	-26.1
D4_Pond	n.a.	-99.0	-96.5	-77.7	-42.5	-25.4
D4_Stream	n.a.	-98.6	-41.3	-80.4	-47.0	-26.8
D5_Pond	-100.0	-100.0	-99.0	-90.5	-53.0	-28.1
D5_Stream	-100.0	-100.0	-72.5	-89.9	-49.6	-8.0
D6_Ditch	-99.3	-99.4	-99.1	-95.5	-65.3	-31.9
R1_Pond	-96.2	-88.2	-82.7	-80.7	-80.0	-79.8
R1_Stream	-92.2	-76.2	-65.2	-61.3	-59.8	-59.4
R2-Stream*	-	-	-	-	-	-
R3_Stream	-100.0	-100.0	-100.0	-99.9	-99.9	-99.9
R4_Stream	n.a.	92757.1	26606.8	18598.4	16401.5	15824.4

n.a. not applicable because the results of FOCUS TOXSWA for winter cereals was below 0.001 µg/L * comparison not possible

Table 31: Relative difference (%) of concentrations for applications to maize instead of winter cereals.

Results of FOCUS surface water scenarios for compounds with low sorption (Kfoc = 30 L/kg) when 1 kg/ha were incorporated 14 days before crop emergence (FOCUS TOXSWA 5.5)

DegT50 (d)	1	3	10	30	100	300
D3_Ditch	n.a.	-100.0	-99.7	-68.7	-25.2	-13.0
D4_Pond	n.a.	-99.9	-99.4	-79.6	-37.5	-17.7
D4_Stream	-99.9	-99.7	-99.6	-83.6	-35.7	-19.5
D5_Pond	-100.0	-100.0	-99.8	-91.9	-46.8	-14.6
D5_Stream	-100.0	-100.0	-99.7	-92.9	-49.0	-12.1
D6_Ditch	-99.7	-99.7	-99.4	-98.4	-81.9	-44.9
R1_Pond	-96.5	-87.9	-81.6	-78.6	-75.8	-74.9
R1_Stream	-92.8	-75.6	-63.0	-58.4	-56.6	-56.1
R2-Stream*	-	-	-	-	-	-
R3_Stream	-100.0	-99.9	-99.6	-99.3	-99.2	-99.2
R4_Stream	n.a.	13282.4	4076.3	2897.7	2570.9	2484.4

n.a. not applicable because the results of FOCUS TOXSWA for winter cereals was below 0.001 µg/L * comparison not possible

Table 32: Relative difference (%) of concentrations for applications to maize instead of winter cereals.

Results of FOCUS surface water scenarios for compounds with moderate sorption (Kfoc = 300 L/kg) when 1 kg/ha were incorporated 14 days before crop emergence (FOCUS TOXSWA 5.5)

DegT50 (d)	1	3	10	30	100	300
D3_Ditch	n.a.	n.a.	n.a.	n.a.	n.a.	239.2
D4_Pond	n.a.	-100.0	-99.8	-89.8	-60.6	-35.7
D4_Stream	n.a.	-100.0	-99.8	-90.2	-61.4	-37.9
D5_Pond	n.a.	-100.0	-93.2	-97.1	-75.1	-50.3
D5_Stream	n.a.	-100.0	14.0	-97.2	-79.3	-56.4
D6_Ditch	-100.0	-100.0	-100.0	-99.3	-93.0	-78.4
R1_Pond	-97.1	-70.5	-23.6	12.8	28.8	948.6
R1_Stream	-94.0	-74.8	-58.5	-52.1	-49.6	394.5
R2-Stream*	-	-	-	-	-	-
R3_Stream	-100.0	-99.1	-88.0	-75.8	-69.2	161.7
R4_Stream	n.a.	1236.4	217.1	111.4	83.6	1554.7

n.a. not applicable because the results of FOCUS TOXSWA for winter cereals was below 0.001 µg/L * comparison not possible

Table 33: Relative difference (%) of concentrations for applications to maize instead of winter cereals.

Results of FOCUS surface water scenarios for compounds with strong sorption (Kfoc = 3000 L/kg) when 1 kg/ha were incorporated 14 days before crop emergence (FOCUS TOXSWA 5.5)

DegT50 (d)	1	3	10	30	100	300
D3_Ditch	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
D4_Pond	n.a.	n.a.	-99.6	-80.6	-44.6	-18.0
D4_Stream	n.a.	n.a.	-99.6	-81.3	-42.5	71.6
D5_Pond	n.a.	n.a.	-100.0	-94.4	-56.8	-45.6
D5_Stream	n.a.	-100.0	-100.0	-94.8	-54.5	-37.9
D6_Ditch	n.a.	-100.0	-100.0	-99.6	-77.1	-56.1
R1_Pond	n.a.	-91.6	-66.5	-47.0	-17.3	43.8
R1_Stream	-94.4	-74.8	-46.0	-18.7	-4.8	0.6
R2-Stream*	-	-	-	-	-	-
R3_Stream	-100.0	-98.5	-74.5	-42.8	-23.8	-21.2
R4_Stream	n.a.	900.6	113.1	37.1	17.1	11.3

n.a. not applicable because the results of FOCUS TOXSWA for winter cereals was below 0.001 µg/L * comparison not possible

Most of the differences shown in Table 30 to Table 33 are negative which means that in maize lower concentrations are simulated than in winter cereals. No comparison was made if the concentrations in winter cereals was below 0.001 µg/L. The minimum value in the table (i.e., -100 %) means concentration of 0 for maize and concentrations above 0.001 µg/L in winter cereals. Though the general trend is that lower concentrations were simulated in maize than in winter cereals there is, however, a significant exception from this trend: The R4 streams scenario in maize gives always higher concentrations than R4 stream simulations when application were done before winter cereals was cropped. The range of differences goes from 11% (Kfoc: 3000 L/kg, DegT50: 300 d, see Table 33) to 92757% (Kfoc: 3 L/kg, DegT50: 3 d, see Table 30). The extreme range can be explained by the different season of application. Obviously, at R4 applications in spring represent worst-case conditions rather than application in autumn. This finding could be a consequence of the short simulation period of only a single year. Therefore, the situation could change after extending the simulation period to 20 years.

2.2.3 New scenario for animals kept under outdoor conditions

There are currently no recommendations how to use the FOCUS models when animals are kept under outdoor conditions on pastures. Nevertheless, FOCUS simulations could be also performed for this situation assuming some input parameters are adapted. Similar as for the intensively reared animals under indoor conditions, the initial concentration in soil is the base for the calculation. PECsoil initial for pasture animals is calculated as follows (EMA 2005):

$$PEC_{soil\ initial} = \left(\frac{D \cdot Ad \cdot BW \cdot SD \cdot Fh}{1500 \cdot 10000 \cdot 0.05}\right)$$

$PEC_{soil\ initial}$	Predicted Environmental Concentration in soil [µg kg^{-1}]
D	Daily dose of the active ingredient [mg kg$_{bw}^{-1}$ d^{-1}]
Ad	Number of days of treatment [d]
BW	Animal body weight [kg$_{bw}$ animal^{-1}]
SD	Stocking density [animal ha^{-1}]
Fh	Fraction of herd treated [value between 0 and 1]
1500	Bulk density of dry soil [kg m^{-3}]
10000	Area of 1 hectare [m^2 ha^{-1}]
0.05	Depth of penetration into soil [m]
1000	Conversion factor [1000 µg mg^{-1}]

As the FOCUS model requires an application rate rather than an initial soil concentration, the following transformation has to be made:

$$AppRate = \frac{PEC_{soil\ initial} \cdot 0.05 \cdot 1500}{Ad \cdot 100000}$$

AppRate	Application rate as input parameter for FOCUS modelling (kg ha^{-1} d^{-1}*)*
$PEC_{soil\ initial}$	Predicted Environmental Concentration in soil [µg kg^{-1}]
Ad	Number of days of treatment [d]
1500	Bulk density of dry soil [kg m^{-3}]
10000	Area of 1 hectare [m^2 ha^{-1}]
0.05	Depth of penetration into soil [m]
100000	Conversion factor [kg ha^{-1} / µg m^2]

The equation also uses *Ad* the number of days of treatment. This is necessary because the FOCUS model requires a daily application. The application rate calculated by the equation has to be repeated for the number of treatment days on the following days. The calculated application rate for surface water or groundwater models describes an average rate for the whole pasture though the real soil load will be rather inhomogeneous dependent where animals leave excreta. However, as the surface water is reached only after run-off or drainage events during which different substance loadings on the pasture are intensively mixed, the assumption of average conditions is valid. The same is true also for the entry to groundwater. The following additional parameter setting is recommended:

- Crop: grass/alfalfa
- Depth of incorporation: 0 (application to the soil surface)
- Application timing: spring application (starting on 1st March) or autumn application (starting on 1st October)

Spring/autumn application means animals are being treated at this time under outdoor conditions. For all other input parameters, the same input can be used as for manure applications (e.g., “granular application” for FOCUS SW).

Some results for FOCUS GW simulations considering spring applications are given in Table 34. They are based on the following input parameters:

- Kfoc: 300 L/kg
- DegT50: 30 d
- Freundlich 1/n (-): 0.9
- Vapour pressure (Pa): 0
- Molecular mass (g/mol): 300
- Water solubility (mg/L): dependent on sorption: 0.3 mg/L
- Days of treatment: 8
- Application rate (kg/ha): 0.125 kg ha^{-1} d^{-1} (total rate 8 * 0.125 kg/ha =1 kg/ha)
- Plant uptake factor (-): 0

Table 34: Results of FOCUS groundwater scenarios for a compound with Kfoc = 300 L/kg and a DegT50 in soil of 100 d when in total 1 kg/ha are applied (FOCUS PEARL 5.5.5, concentrations in µg/L)

DegT50 (d)	Grass scenario for pasture animals spring	Maize scenario for manure applications spring	Grass scenario for pasture animals autumn	Winter cereals scenario for manure applications autumn
Châteaudun	0.525	1.378	0.618	0.771
Hamburg	1.426	3.513	1.790	5.001
Jokioinen	0.218	-	0.288	1.591
Kremsmünster	0.789	3.111	0.976	4.186
Okehampton	1.301	4.853	1.734	6.797
Piacenza	1.202	2.832	1.754	2.538

DegT50 (d)	Grass scenario for pasture animals spring	Maize scenario for manure applications spring	Grass scenario for pasture animals autumn	Winter cereals scenario for manure applications autumn
Porto	0.508	0.803	0.969	1.804
Sevilla	0.027	0.006	0.036	0.000
Thiva	0.192	0.367	0.316	0.169
Average	**0.708**	**2.108**	**0.942**	**2.540**

The results in Table 34 demonstrate that significantly lower concentrations are to be expected in grass/alfalfa than for two annual crops winter cereals and maize, at least for this compound. However, the general trend with regard to the ranking of concentrations for the different locations is similar. Though the results may be different for different compounds it shows that also the FOCUS grass/alfalfa scenario gives reasonable results and could be used for the risk assessment when animals are kept under outdoor conditions.

2.3 Consideration of risk mitigation methodologies

2.3.1 Introduction

A critical review of the adequacy/appropriateness of risk mitigation measures for veterinary compounds can be found in EMA (2011). These risk mitigation measures are included in the product literature, (i.e. summary of product characteristics (SPC)s and package leaflet) of products for which a risk to the environment was identified with the intended purpose of reducing the risk. This EMA reflection paper is based on the experience gained when formulating risk mitigation measures in line with the criteria specified in the VICH-TGD (EMEA 2008). EMA (2011) mentions minimum distances to surface water when spreading manure from treated animals as a measure "not under control of the veterinarian or animal owner". This measure does not specify if the area between the manured field and the water body is vegetated or not.

This measure on "minimum distances to surface water" is the same as what is currently done in the final step of the FOCUS surface water risk assessment. Originally, the FOCUS surface water models only consisted of three steps without any additional risk mitigations methodologies (FOCUS 2001). However, for the risk assessment of pesticides it was necessary to include a final step where additionally risk mitigation methodologies can be considered. Basically, drift mitigation (buffer zones, special nozzles) and run-off mitigation (vegetated buffer strips) are considered at step 4. Drainage mitigation options are not offered. For veterinary compounds only run-off mitigation is of relevance since for all FOCUS SW simulations the application type "granular application" is used which assumes no drift entries into surface water.

Run-off mitigation can be considered by including vegetative buffer zones between the agricultural field and the water body. No run-off mitigation is suggested in case of strips without vegetation (e.g. field lanes).

Dependent on the width of this buffer zone the transport of water and sediment is reduced. In the simulations, substance entries are reduced in relation to the reduction of water and sediment. Two different strategies for calculating the reduction are used:

- Constant reduction factors dependent on the width of the buffer strip (reduction independently on the run-off/erosion event). The factors are suggested by the FOCUS landscape and mitigation group (FOCUS 2007). Respective factors are available for 10 m and 20 m buffer widths.

- Reduction factors calculated with the mechanistic model VFSMOD. The factors are dependent on various parameter such as the width of the buffer strip, the run-off event and the soil conditions (e.g., moisture) on the buffer strip. VFSMOD is able to calculate reduction for every distance (not only 10 m and 20 m).

Table 35 shows the constant reduction factors dependent on the width of the buffer zone as recommended by FOCUS (2007). The reduction factors are based on field experiments where the effect of the buffer widths was quantitatively determined. The values in Table 35 represent the 90th percentile of the experimental reductions (i.e., in 90% of the experiments the actual reduction factors were higher than the numbers in Table 35).

Table 35: 90th percentile worst-case values for reduction efficiencies for different widths of vegetated buffers and different phases of surface runoff (FOCUS 2007)

Buffer width (m)	10 – 12	18 – 20
Reduction in volume of runoff water (%)	60	80
Reduction in mass of substance transported in aqueous phase (%)	60	80
Reduction in mass of eroded sediment (%)	85	95
Reduction in mass of substance transported in sediment phase (%)	85	95

When using constant reduction factors based on FOCUS (2007) it is assumed that the vegetated buffer will reduce the volume of water or the mass of eroded sediment and the substance mass to the same extent. That means the substance concentrations are not reduced but the extent of the run-off/erosion event. Because of that a reduction of 60% in the substance mass does not mean 60% reduction of the concentration in the receiving water body.

The situation is explained in following example:

Volume of the water body: 100 L

Volume of run-off water: 100 L

Compound mass in run-off water: 1 g

Substance concentration in run-off water: 10 mg/L

Concentration in water body without mitigation: 1 g / (100 L + 100 L) = 5 mg/L

Reduction factor for volume and mass by mitigation 60%

Volume of run-off water considering 60% reduction: 40 L

Compound mass in run-off water considering 60% reduction: 0.4 g

Concentration in water body including mitigation: 0.4 g / (100 L + 40 L) = 2.86 mg/L

Reduction of concentration due to mitigation: 100 · (5 mg/L - 2.86 mg/l) / 5 mg/L = 42.86%

In this example, the reduction of 60% for run-off volume and compound mass lead to a reduction of only 42.86% (not 60%) for the concentration in the surface water body (e.g., the ditch).

The final step can be easily performed using the software SWAN if standard FOCUS simulation results are available. This software supports the user modifying existing Step 3 output of PRZM (i.e., run-off entries) for the step 4 run. SWAN also updates the TOXSWA input files so that the surface water model will use the modified PRZM output. SWAN also provides both options (constant reduction factors and event dependent reduction based on VFSMOD). It is currently planned to establish SWAN as an official FOCUS model at the FOCUS website.

2.3.2 Results simulations including mitigation

In this section results of step 4 simulations with both options and buffer zones of 10 m and 20 m are presented to demonstrate the effect of this mitigation options for veterinary compounds (see Table 36).

Table 36: Effect of different mitigation options for FOCUS surface scenarios when 1 kg/ha were incorporated (FOCUS TOXSWA 5.5, Begin of application window: 14 days before crop emergence of maize, Kfoc: 300 L/kg, DegT50: 100 d, concentrations in µg/L)

Buffer width (m)	No mitigation	10 – 12 FOCUS	10 – 12 VFSMOD	18 – 20 FOCUS	18 – 20 VFSMOD
R1_Pond	0.064	0.026	0.004	0.013	0.000
R1_Stream	2.413	1.081	0.031	0.563	0.000
R3_Stream	3.177	1.450	0.983	0.761	0.694
R4_Stream	1.831	0.827	0.001	0.432	0.000

When using FOCUS (2007) reduction factors, the results show that mitigation reduces concentration by about a factor of 2 or 4 for buffer widths of 10 m and 20 m, respectively. This is nearly independent of the location. In contrast, the reduction calculated by VFSMOD is event dependent and consequently depends highly on the weather at the locations. This leads to drastic reductions at R1 and R4 whereas the concentrations at R3 are similar as with constant reduction factors. Generally, the reduction factors recommended by FOCUS (2007) are more conservative than the results of VFSMOD. The D (=drainage) scenarios are not mentioned in Table 36 because no FOCUS mitigation is possible for this kind of scenarios, where the water (incl. active compound) enters the surface water body belowground.

2.4 Modelling ionising substances

2.4.1 Introduction

Many veterinary compounds are ionising substances. The consequence is that the standard assumption of strong correlation of organic carbon content in soil and sorption does not work. Guidance how to consider this type of substances in the risk assessment is given EMA (2018). In those cases, the lowest or the most appropriate adsorption coefficient should be used. In the following chapter some advice is given how these substances could be handled when performing FOCUS GW and SW simulations.

2.4.2 Impact on FOCUS GW simulations

FOCUS assumed implicitly that the sorption of substances is correlated to the organic matter or organic carbon content. Therefore, substances whose sorption is correlated to other soil properties (e.g. pH, sesqui-oxides or clay minerals) may need evaluation outside the standard exposure assessment. At least, the FOCUS GW report (FOCUS 2009) gives recommendations how to consider special substances where sorption is dependent on pH in soil. PEARL is able to consider the pH-dependency. The internal model in PEARL assumes that the phenomenon is caused by different fractions of the ionised and the non-ionised form dependent on the pH in soil. The user has to enter the “pure” Kfoc for both forms. In the PEARL shell they are used as “Kom acid” and “Kom base”. For estimating the fraction dependent on the pH the pKa has to be entered. The pKa determines at which pH there is equal distribution between the two forms. Finally, a pH-correction can be entered. This can be useful because the sorption of pesticides is often measured in a 0.01 M CaCl2 solution. If the soil pH has been measured in a different way (e.g. pH-KCl), a correction may be required. There is a small tool available where the necessary parameters can be obtained:
https://www.bvl.bund.de/SharedDocs/Downloads/04_Pflanzenschutzmittel/Input_Decision_3.xlsm;jsessionid=6AA5491CE4318DB7DAE63408BBFDB573.2_cid372?__blob=publicationFile&v=3

An example how pH-dependent sorption may influence the concentrations in groundwater is given in the following Table 37. Following assumptions are made for the calculations:

- Kfoc of the acid form (non-ionised): 300 L/kg (KOM: 174 L/kg)
- Kfoc of the base form (ionised): 3 L/kg (KOM: 1.74 L/kg)
- DegT50: 100 d
- pKa: 4.5

As in the previous sections 1 kg/ha of the substance is applied in winter cereals 14 days before emergence of the crop. In Table 37 also the results for two “normal” compounds are presented with Kfoc of 300 L/kg and 3 L/kg, respectively.

Table 37: Results of FOCUS groundwater scenarios for three compounds (all with DegT50s of 100 d) when in total 1 kg/ha are applied in winter cereals 14 days before crop emergence (FOCUS PEARL 5.5.5, concentrations in µg/L)

DegT50 (d)	Top soil pH of the scenario	Kfoc = 3 L/kg	Special substance with Kfoc varying between 3 L/kg and 300 L/kg	Kfoc = 300 L/kg
Châteaudun	8.0	358.636	337.900	0.771
Hamburg	6.4	498.078	251.555	5.001
Jokioinen	6.2	602.628	309.269	1.591
Kremsmünster	7.7	226.603	216.880	4.186
Okehampton	5.8	223.879	157.966	6.797
Piacenza	7.0	251.394	193.618	2.538
Porto	4.9	175.611	13.948	1.804
Sevilla	7.3	132.310	112.709	0.000
Thiva	7.7	382.960	356.643	0.169
Average	6.6	311.683	201.574	2.761

The results in Table 37 show that the simulated concentrations for the "ionasible" substance are always found to be between respective results of the "normal" substances. At least for this example, concentrations are close to the results of the low Kfoc of 3 L/kg i.e., the Kfoc of the ionised form of the "special" substance. The lower the pH in soil the more dominant the non-ionised form in soil becomes. That leads to relatively small differences to the high sorbing compound Kfoc of 300 L/kg (e.g., location Porto).

Obviously, PEARL is able to simulate reasonable concentrations in groundwater dependent on the pH of the location. Though this procedure is a valid transformation of the behaviour of ionising substances to other pH values it may nevertheless violate the original definition of the FOCUS locations as worst-case scenarios. Background is that the soil pH values were never used as a selection criterion in the development and may therefore also not represent worst-case conditions (as e.g., organic carbon contents or the climatic conditions) in soil. Therefore, as a simple, practical and conservative strategy also a simulation based on the worst-case sorption constant in the laboratory study could be used for the risk assessment.

The same worst-case strategy could be considered also when the sorption constant is correlated to other soil parameters (e.g., the clay content) or the DegT50 is pH-dependent.

2.4.3 Impact on FOCUS SW simulations

The FOCUS SW report (FOCUS 2001) does not discuss the problem of ionising substances. Independent whether sorption is found to be correlated with organic carbon in soil or whether Kfoc/DegT50 are pH-dependent the mean values should be considered for the simulations.

However, it may be more appropriate to consider worst-case selections (e.g., minimum Kfoc, maximum half-life) in case the sorption constant is clearly not correlated to the organic carbon content or the DegT50/Kfoc is pH-dependent. That would be at least a reasonable worst-case selection. The extent of the change in concentration when picking the worst-case instead of the average value can be taken from respective simulation results in section 2.1.3.

3 Potential problems when performing simulations

3.1 Problem description

In some cases, different model users could not reproduce their results though all input parameters seemed identical. In this chapter, possible causes for this problem are discussed. All FOCUS models are deterministic. Therefore, any differences in results are caused by the use of input parameters. To reduce these problems this chapter focuses on parameters which are not clearly defined and are also to some extent hidden in the shell.

In addition, the use of different computers systems (windows version, regional settings, e.g., date format, decimal point/comma) is an important point to consider. Before using the FOCUS models, the user should check that the decimal point is selected when expressing numbers.

All these problems mainly occurred when using the FOCUS surface water scenarios (SWASH package).

In addition, in some cases the refined PEC calculated by the FOCUS models was also higher than the initial PECsw from the Tier A equations.

Dummy data tests including respective model results are provided in the FOCUS models. They can be used by all model users. That should help users to perform the simulations and increase confidence in the model results. Additional dummy data sets have recently been published by EMA 2022.

3.2 Input parameters not clearly defined in current guidance.

The problem is purely related to FOCUS surface water simulations. Principally, problems could be caused either by using different properties of the compound or by entering a different application scenario. In the following both types of problems are discussed. However, it is expected that most of the problems occur because of different application setting.

3.2.1 Substance specific input parameters

Only a limited number of substance specific input parameters has to be entered by the user (e.g., Kfoc, DegT50, Freundlich exponent, water solubility, vapour pressure). There are, however more input parameter set with FOCUS default values in SWASH. These input parameters (e.g., molar enthalpy of dissolution) are hardly ever changed which is also in line with EMA guidance. The only exception is the "coefficient of update by plants (TSCF)" which can be found in the tab "crop processes". The FOCUS default value is 0.5 whereas the recommended EMA value for this parameter is 0.0. It may happen that users unintentionally keep the FOCUS default value (0.5) which may lead to different results compared the correct setting of the TSCF (0.0).

3.2.2 Input parameters related to the application

There are several parameters, which were not clearly defined in the current guideline. They are related to the application method, the chemical application method (CAM), the incorporation depth, and the application window. In the following, these parameters are explained and possible causes for errors are discussed.

- Application method:
  Four different types can be selected here. "Aerial application" and "ground spray" are not

relevant for veterinary compounds. They refer to spraying of pesticide. If selected the model will consider crop dependent spray drift emissions into surface water. The other options "granular" and "soil incorporation" are principally relevant for veterinary compounds. Though the guidance recommends "granular" sometimes "soil incorporation" may have been selected by users which later led to differences in results.
It is important to realise that PRZM is not sensitive to this parameter. Independent on the setting (granular or soil incorporation) the same results will be obtained. MACRO however, is very sensitive to the selection. The background can be explained as follows:
Soil incorporation means that the compound is placed into the soil matrix and possible transport through macro pores is limited. If, however, granular is selected the compound is placed outside the soil matrix and substances are transported through macro pores to a much higher extent. Technically, it is the parameter ZMIX (mixing depth) which is very small when soil incorporation is selected. The consequence of the different ZMIX for the two options are always higher concentrations in the surface water when using "granular application" instead of "soil incorporation". According to the EMA guideline "*granular application is the closest scenario to manure spreading*" and is to be used. a discussion on the best option for the application method is out of the scope of this draft document.

- Chemical application model (CAM):
This parameter is only used by PRZM. This model has several options how the substance is mixed in the soil. As the guidance is not specific here, different setting of this parameter may lead to different results. The recommended option would be CAM=4 which means same concentration in the incorporated layer. However, the shell lists all possible options which are:

  - Application soil linear (CAM=1): to be considered for sprayed applications, not suitable when substances are incorporated
  - Incorporation soil uniform (CAM=4): same concentrations in the incorporated layer
  - Incorporation soil linear increase (CAM=5): linear increase from top to bottom of the incorporated layer
  - Incorporation soil linear decrease (CAM=6): linear decrease from top to bottom of the incorporated layer
  - Incorporation soil at one depth (CAM=8): the compound is placed at a single depth in soil (most suitable for pesticides that are injected rather than incorporated)

- Incorporation depth:
Similar as the chemical application model also the incorporation depth is only sensitive to PRZM. If the incorporation depth is increased lower concentrations can be expected for the surface water body. Unfortunately, no details are given in the EMA guidance which depth should be used for R scenarios. The FOCUS guidance from 2000 recommends incorporation over 20 cm for annual crops (such as winter cereals) where ploughing is considered. This would be an acceptable number also for veterinary compounds. According to EUROSTAT data from 2016, conventional tillage takes place on about 2/3 of arable land on EU average (EUROSTAT 2016). The value of 20 cm is however not suitable for situations when the soil is not ploughed e.g., permanent crops or conservation agriculture. The share of conservation agriculture differs regionally and can be up to > 65 % of arable land in some regions such Eastern Germany or parts of Portugal. In addition, 5 cm are also the appropriate value for

grassland. The use of 5 cm as realistic worst-case for FOCUS surface water is also supported by recent research of Haupt et al. (2022) for the situation in Germany.

- Application window:
For all applications within a year an application window must be given in which applications are principally possible with regard to the season or crop development. An additional tool called PAT (pesticide application timer) in the SWASH package takes care that actual applications are always placed on days which are reasonable according to the weather in the scenario (e.g., no extreme rainfall during application dates). That means it is not possible for the user to enter directly an application date. There is no guidance given about the window by EMA. However, the FOCUS default application window (begin of the window 14 days before crop emergence) is not in contraction to the requirements for manure applications (before drilling of the crop). Therefore, it is best to keep the default setting here, to guarantee that different users come to the same concentrations in surface water as changes of this value need to be done for every scenario manually and are prone to mistakes. Within the next release of the software the simulation period will be extended to 20 years and the dominance of a single application dates for the risk assessment will be reduced (EFSA 2020). The release will also include a less complicated PAT (pesticide application timer).

4 Manual for FOCUS simulations

4.1 Groundwater simulations

As already described in previous chapters the FOCUS scenarios were originally developed for pesticides. This is the reason why the shell and some of the input parameters incl. default values are not always in line with the needs in the risk assessment for veterinary compounds. However, this does not discredit the application of PEARL for veterinary compounds. The assumptions used in the model (chromatographic transport through the soil passage using the convection dispersion equation with sorption to organic carbon as key process) are valid also for other compounds as pesticides. It is just the design of the existing shells which are not perfectly designed for the risk assessment of veterinary compounds.

In this manual the differences to the pesticide input parameters settings are explained and how successful simulations can be performed for veterinary compounds.

4.1.1 Downloading FOCUS PEARL

The software can be downloaded from the FOCUS website which is currently hosted by JRC. The current link to the FOCUS groundwater models is

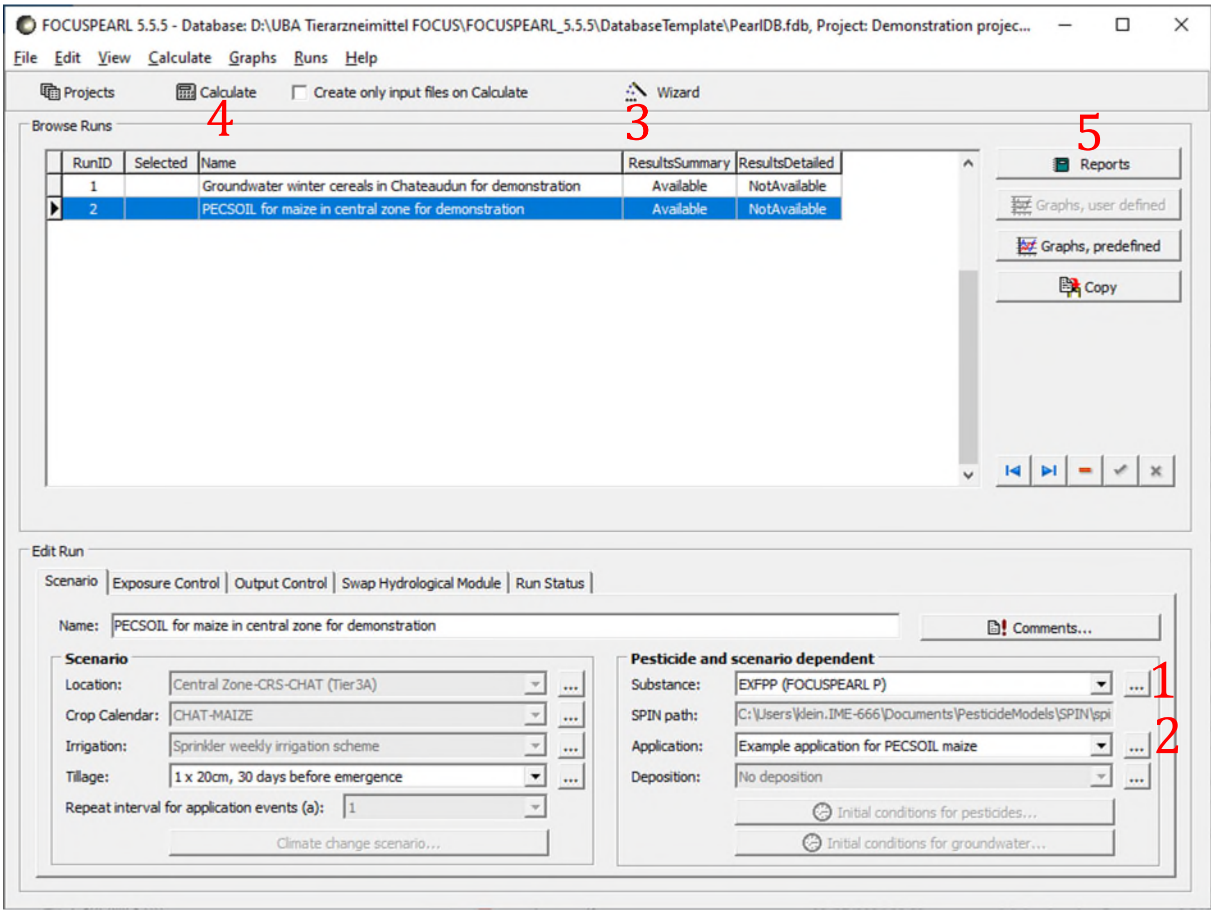
https://esdac.jrc.ec.europa.eu/projects/ground-water

Please consider that FOCUS Users have to install also FOCUS_SPIN_3.3 as PEARL v 5.5.5 itself does not store substance properties. This should be done before installing PEARL v 5.5.5. SPIN has to be installed on a local (and not network) drive. The default directory for installing the SPIN application is C:\Program files (x86)\Pesticide Models\SPIN on a 64 bit platform or C:\Program files\Pesticide Models\SPIN on a 32 bit platform. It should be noted that SPIN version 3.3 facilitates the use of both FOCUSSWASH 5.3 and FOCUSPEARL 5.5.5. To avoid problems by modifying the properties of a substance using one application while the other application is running at the same time, only one application at the time can have access to the SPIN database. The user has to exit from the application that has a connection to the SPIN database before the other application using SPIN can be started.

4.1.2 General Principles

After clicking at the FOCUS PEARL icon, the model presents a form where all runs of the last project are presented (see Figure 1). In order to run simulations a fixed sequence has to be followed which is explained further below.

Figure 1: FOCUS PEARL: Overview on simulations in the project



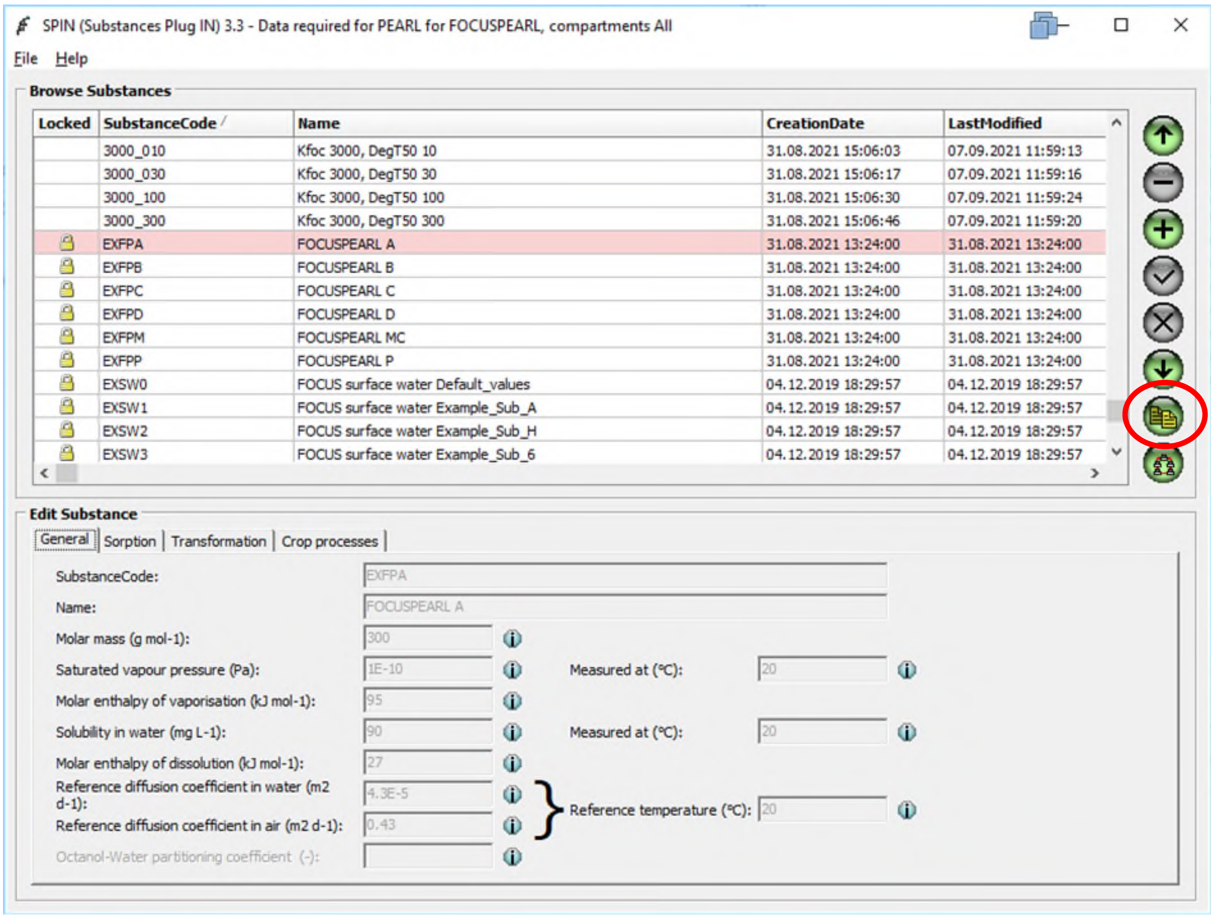
The numbers in Figure 1 refer to the different steps.

1) Enter substance specific parameters (e.g., sorption, degradation data)
2) Enter application data (e.g., application rate)
3) Define the project (e.g., which locations should be included in the assessment)
4) Start the simulation
5) Evaluate the results

4.1.3 Editing substance input parameters

In the first step the substance parameters should be entered. The form in Figure 2 opens after clicking at the respective button in the initial form of PEARL (see the “1” in Figure 1).

Figure 2: FOCUS PEARL: Editing general substance parameters



Next you should copy one of the default substances (e.g., “EXFPA”) using the copy button (see the red circle in Figure 2). This has an advantage compared to creating a new substance since most of the default values are already correctly set.

In the tab “General” enter the substance code and the name.

Furthermore, enter the values for following parameters:

- molar mass
- vapour pressure
- water solubility

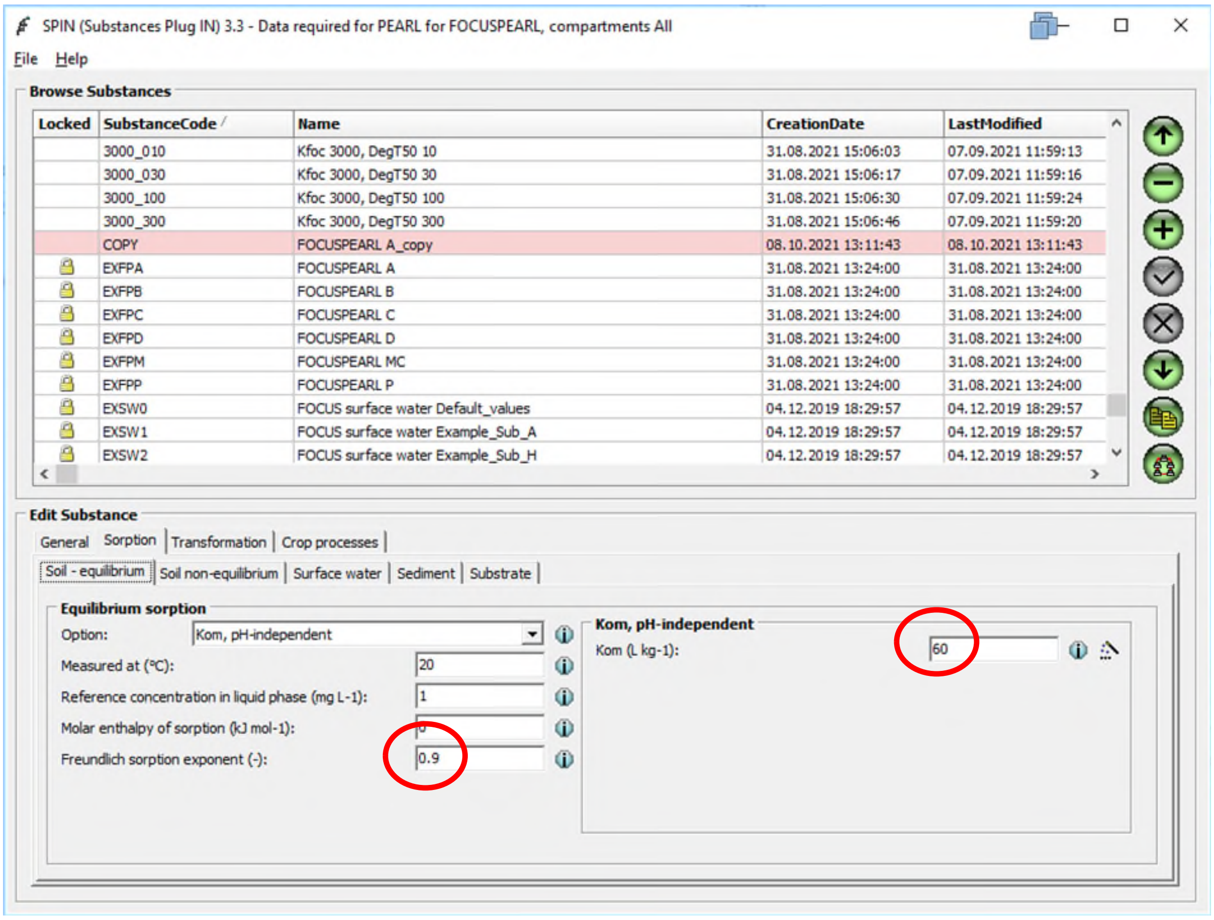
These three input parameters are only used to estimate Henry’s law constant and the soil concentrations of compounds in the air compartment. As a conservative assumption the vapour pressure could be set to zero. Then the water solubility will have no influence at all and the concentrations in air will be set to 0 for all compartments. The remaining fields are set with correct default values.

Now, enter the sorption parameters in the tab “Sorption” (see Figure 3). Currently, only

- Kom
- Freundlich sorption coefficient

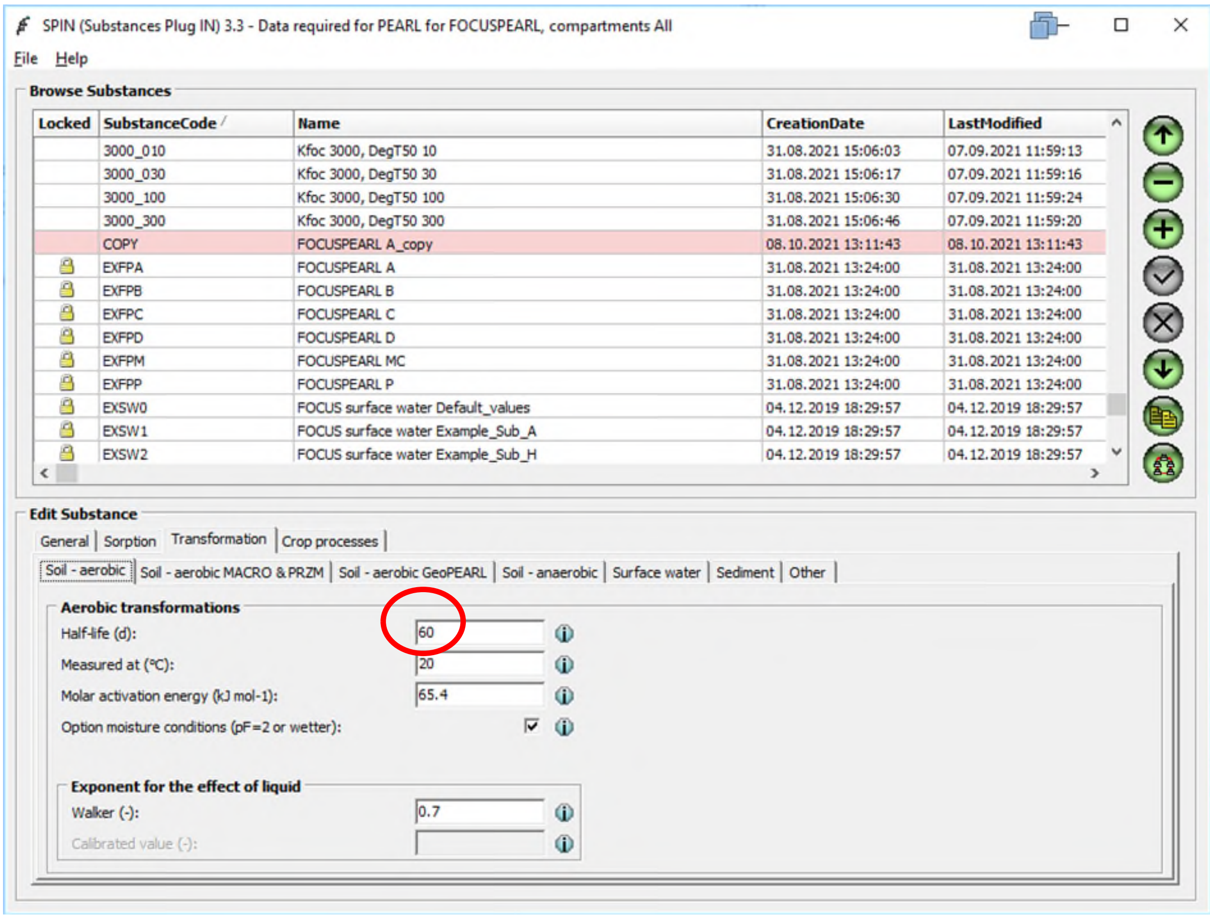
in the sub-tab "soil – equilibrium" have to be filled. The remaining fields are set with correct default values. With regard to the correct setting of the Freundlich exponent it is mainly recommended to use the arithmetic mean (see EMA 2022 for further details). For the Kom the geometric mean should be considered if sorption is mainly related to organic carbon and at least 5 soils have been tested (EFSA 2014, EMA 2018). If instead of the Kom only the Koc is available the shell includes a wizard which allows the transformation of Koc values into Kom values.

Figure 3: FOCUS PEARL: Editing sorption parameters



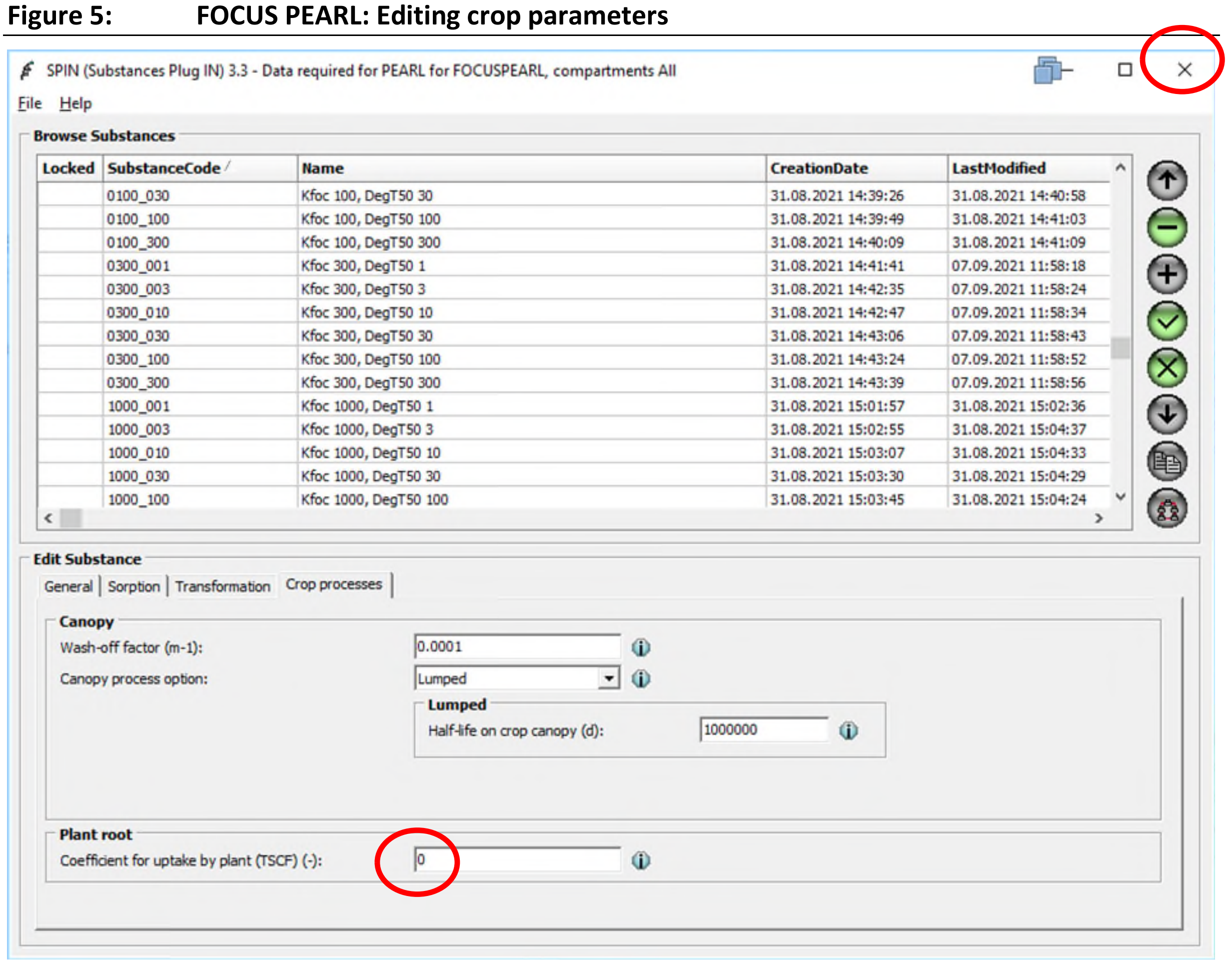
Then, the degradation parameters have to be entered in the tab "Transformation" (see Figure 4). Only a single field the half-life at 20 °C have to be entered (red circle in Figure 4). All other parameters are set with correct default values. According to EMA (2018) soil biodegradation should be carried out using four different soils. In a study where four soils have been used it is acceptable to use the geometric mean DegT50 value in the risk assessment. The studies should be evaluated based on the recommendations of FOCUS (2014). That means they should be analysed using simple first order and biphasic kinetics. If during the study biphasic behaviour is observed a suitable first order rate constant must be deduced based on the recommendations of FOCUS (2014) since PEARL can only handle first order kinetics.

Figure 4: FOCUS PEARL: Editing degradation parameters



Now, the crop parameters have to be entered in the tab "Crop processes" (Figure 5). Again, only a single field, "the coefficient for uptake by plants", is relevant. It is important that this parameter is set to "0" by default. Unfortunately, the PEARL model uses a default of 0.5 here, which is common value for pesticides (see red circle in Figure 5).

Figure 5: FOCUS PEARL: Editing crop parameters



When all these substances specific inputs have been given, the form can be closed using the x-button in the top right corner of the form (see Figure 5).

4.1.4 Editing application input parameters

In the second step the application parameters should be entered. The form in Figure 6 opens after clicking at the button (see the "2" in Figure 1).

In order to create a suitable data set click at the "+" button (see the red circle in Figure 6), enter some information in the field "code" and "description" and accept the changes (see the red rectangle in Figure 6). Now the concrete application scenario has to be defined. When veterinary compounds are applied with manure the application date should be 14 days before crop emergence. Such a scheme can be defined using relative applications (click at the "+" bottom, i.e., red triangle in Figure 6 to define a record) and enter the relevant information in the bottom right part of the form (see Figure 7).

Figure 6: FOCUS PEARL: Editing application parameters

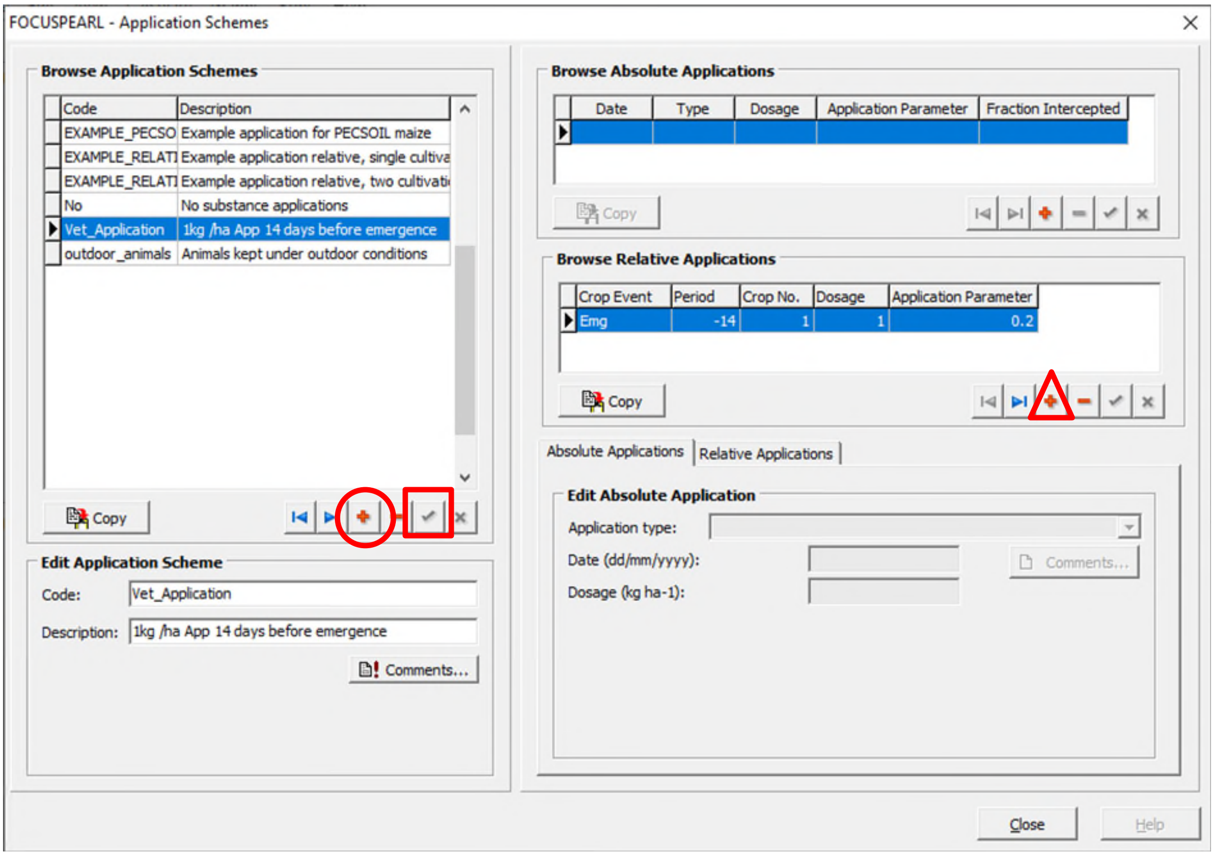
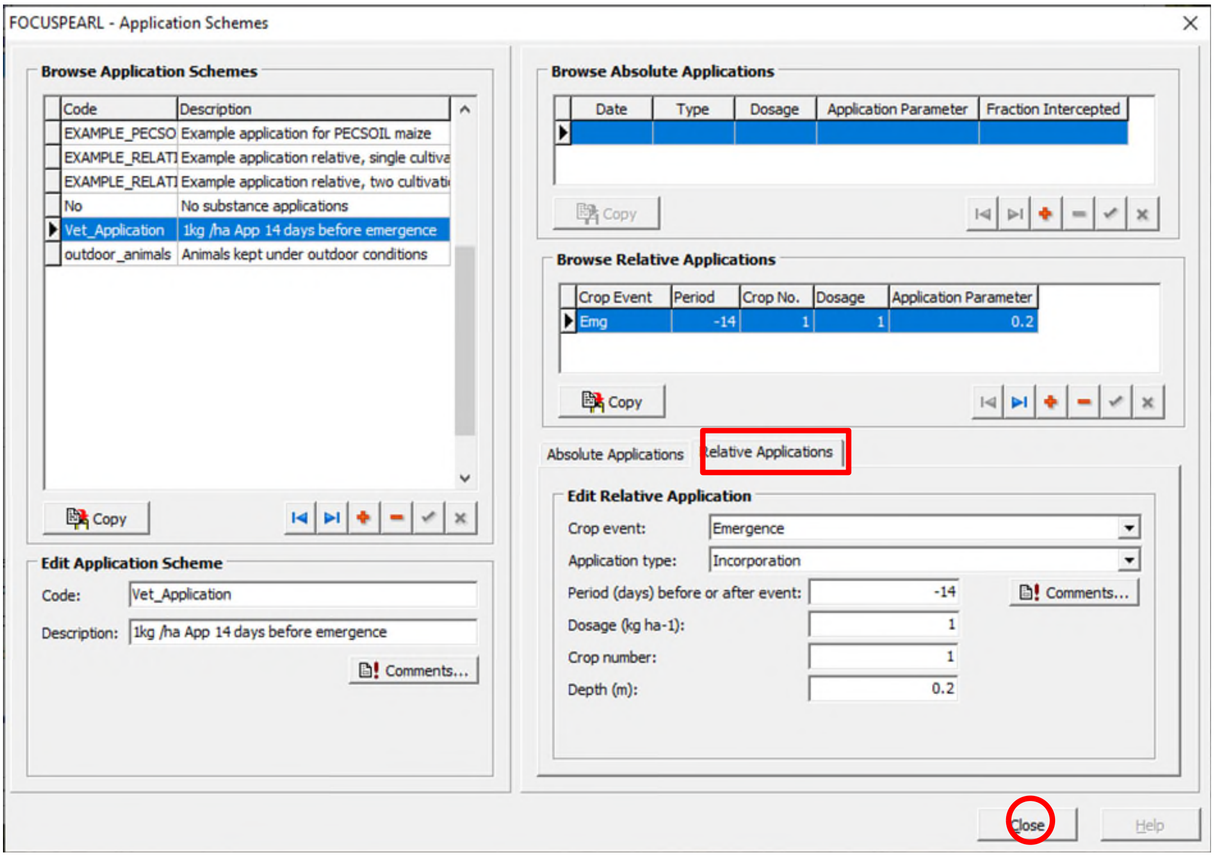


Figure 7: FOCUS PEARL: Editing application parameters



After clicking at the "relative application" tab (see red rectangle in Figure 7) enter the necessary information:

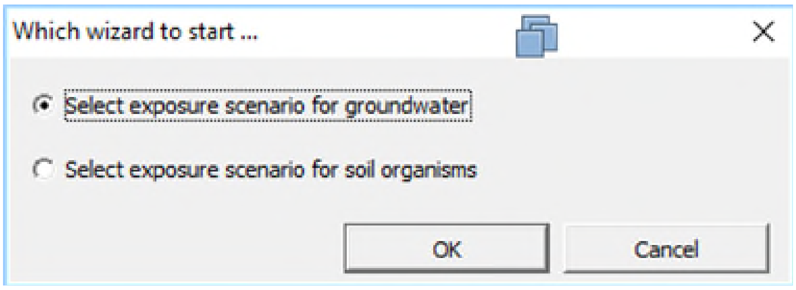
- Crop event: Emergence
- Application type: Incorporation
- Period: -14
- application rate: your dosage in kg/ha
- Crop number: 1 (default)
- Depth (m): 0.2 (worst-case compared to 0 or 0.05 cm)

The dosage can be easily calculated based on PECsoil according to EMA (2005). Then, all information about the application pattern has been given and the form should be closed using the close bottom (see red circle in Figure 7). Principally, also absolute applications could be used here, but relative applications are fail-safe when more than one location is to be simulated.

4.1.5 Defining the project

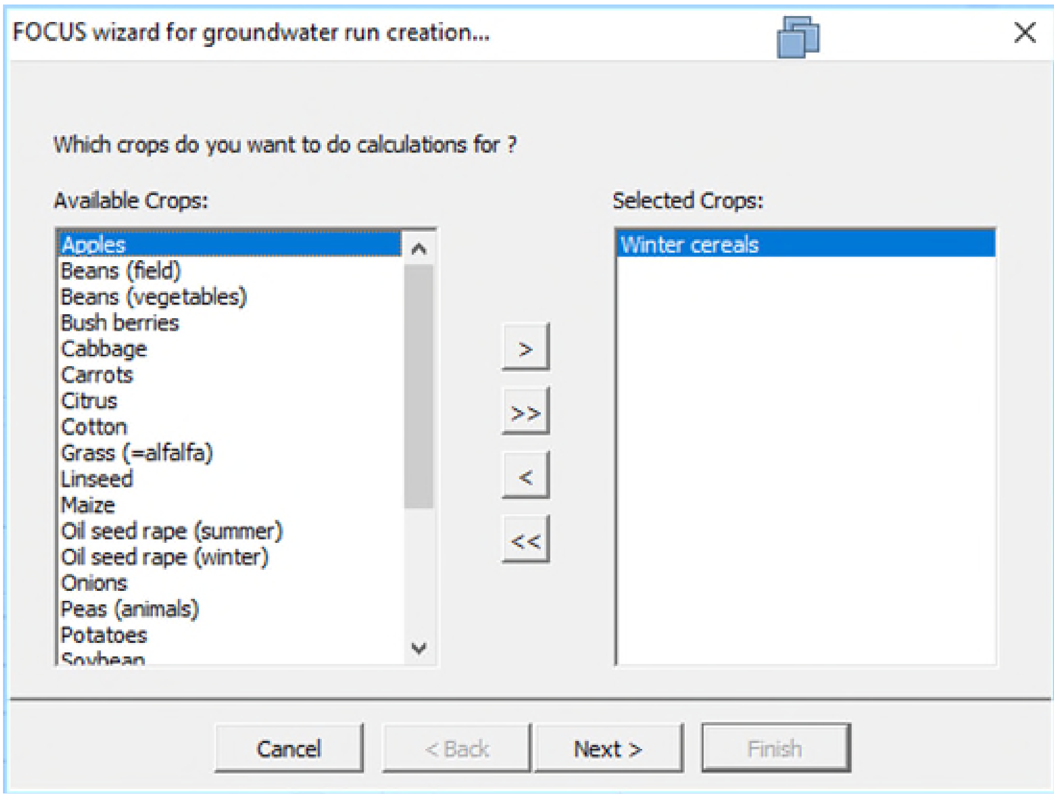
In the next step the project should be defined. The form in Figure 8 opens after clicking at the button "Wizard" (see the "3" in Figure 1).

Figure 8: FOCUS PEARL 5.5.5: Defining type of scenarios



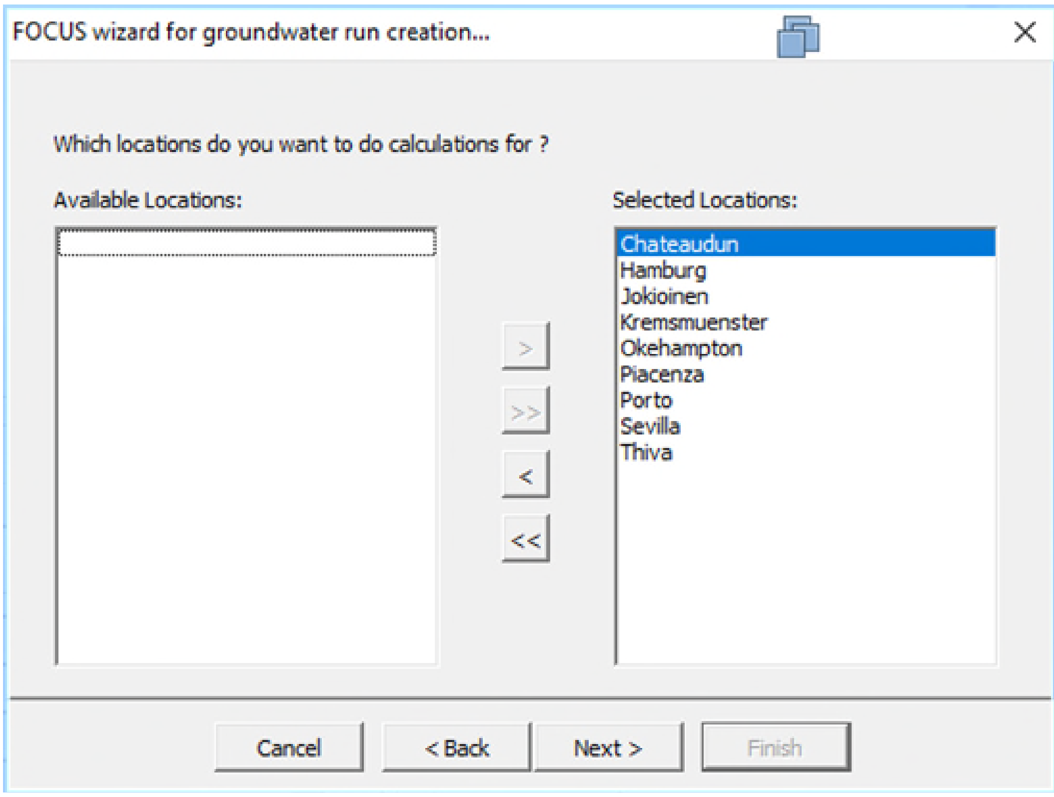
Always the (preselected) groundwater simulations have to be accepted here. Then the form presented in Figure 9 is shown. Please select the crop you want to simulate (normally: winter cereals) and continue with the next step.

Figure 9: FOCUS PEARL 5.5.5: Defining the crop for the simulation



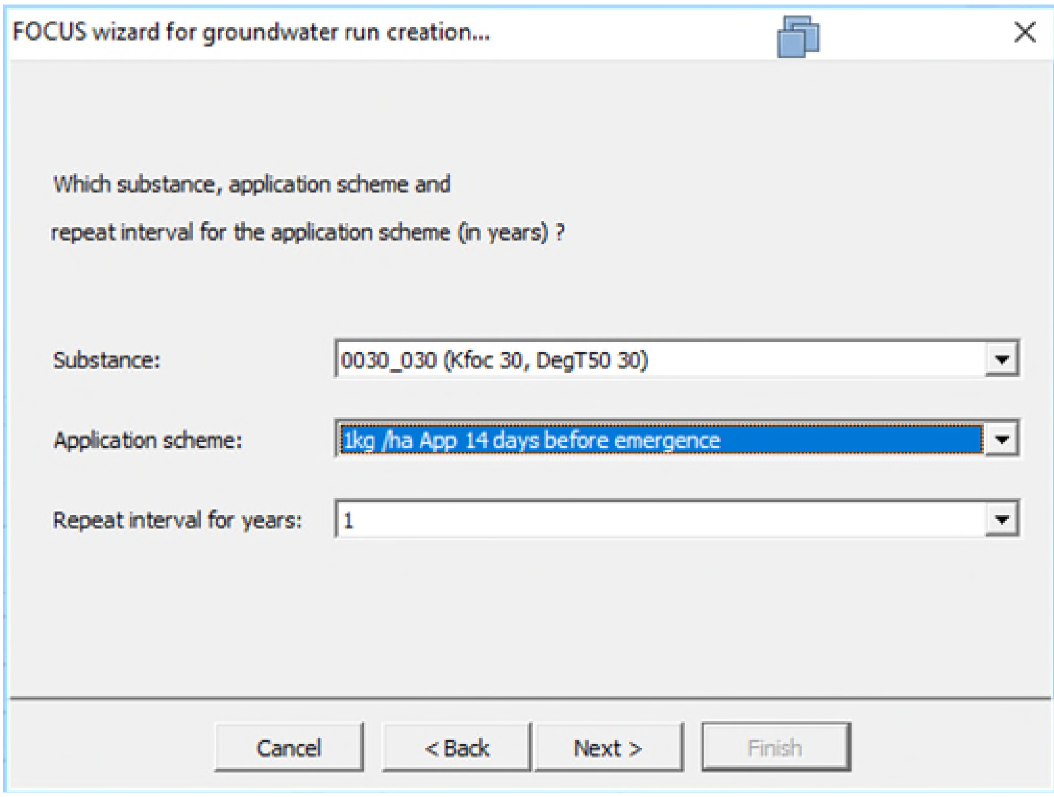
Now, the locations for the simulations are presented (see Figure 10). The recommendation from the EMA GL is Okehampton. Other locations can be chosen as applicable. According to the results presented in 2.1.2 for low sorbing compounds (Kfoc = 1 L/kg) Hamburg and Jokioinen are the worst-case locations, whereas for moderately (Kfoc = 100) and strongly sorbing compounds (Kfoc = 1000 L/kg) Hamburg and Okehampton showed maximum concentrations.

Figure 10: FOCUS PEARL 5.5.5: Defining the locations for the simulation



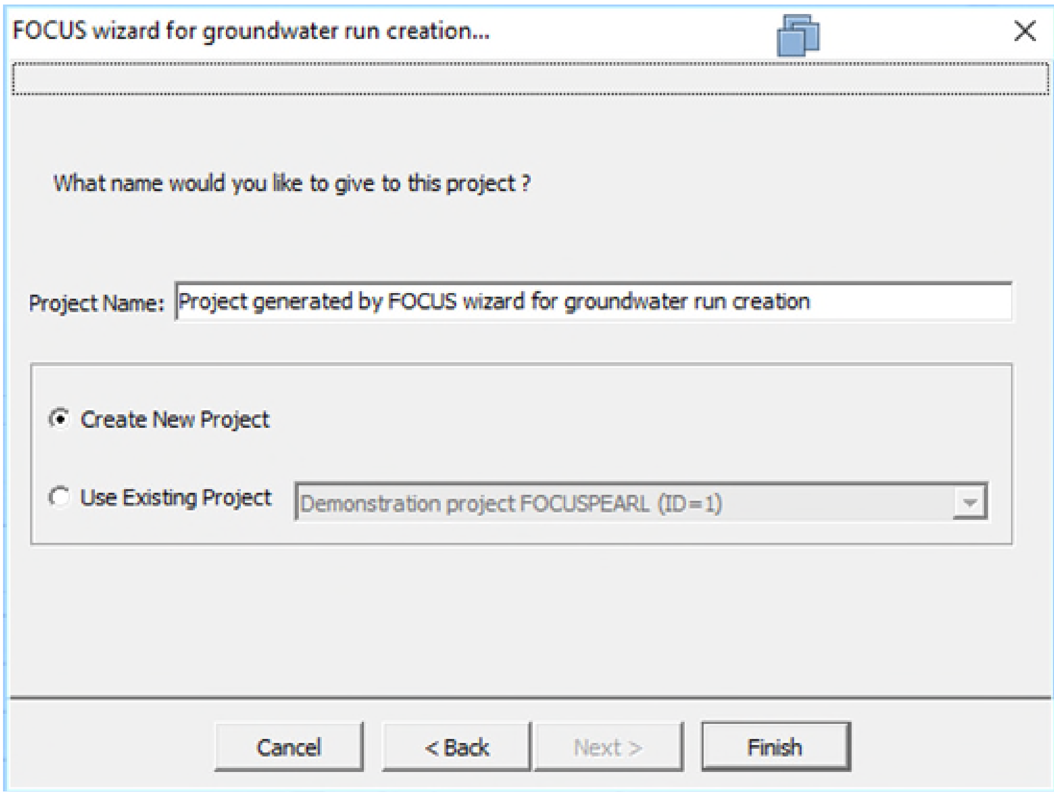
After the next button was clicked the substance and the application scheme have to be picked. For the application scheme pick the record with applications 14 days before emergence. This represents the default for veterinary compounds (see Figure 11). The repeat interval should be set to “1” which means applications every year.

Figure 11: FOCUS PEARL 5.5.5: Selecting substance and application scheme



In the final step the new project should be created and then named (default option, see Figure 12). Alternatively, the simulations could be added to an existing project.

Figure 12: FOCUS PEARL 5.5.5: Naming the project

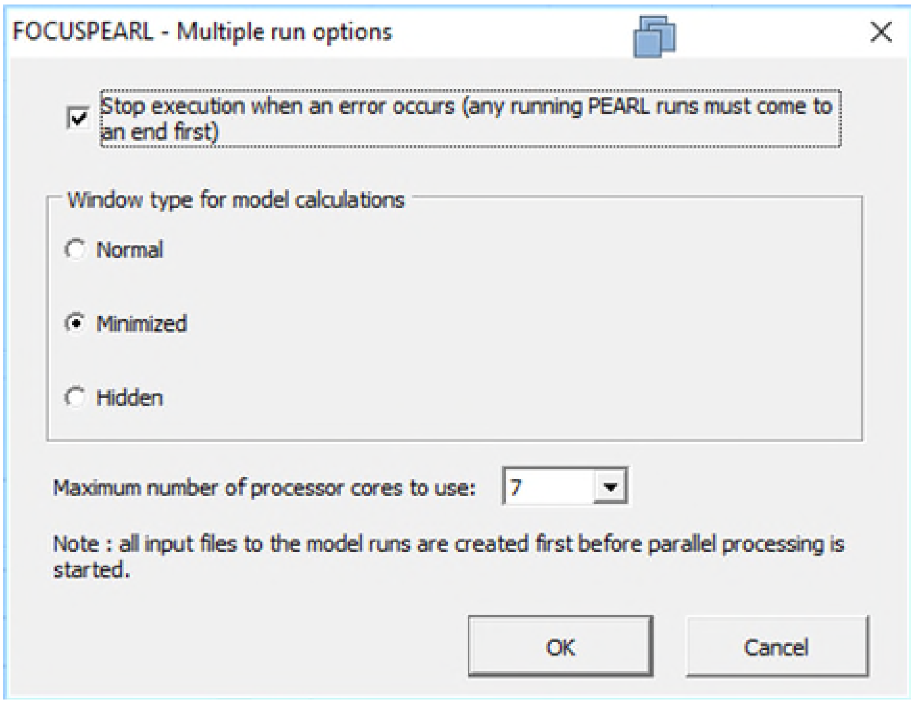


After having clicked at “Finish” the project will be created.

4.1.6 Running the project

At this stage the simulation can be started. Only the selected entries in this form are considered for the simulations. After a click at the “Calculate” button (see the “4” in Figure 1) a form with several options is loaded (see Figure 13). Most relevant is the last option, the “Maximum number of processor cores to use”. Dependent on the number here, parallel PEARL runs will be started in order to save time. If e.g., 9 single runs have been added to the project and the number of cores considered by PEARL is 3, then PEARL will run three simulations in parallel and the results will be obtained 3 times faster than with only a single PEARL run at a given time.

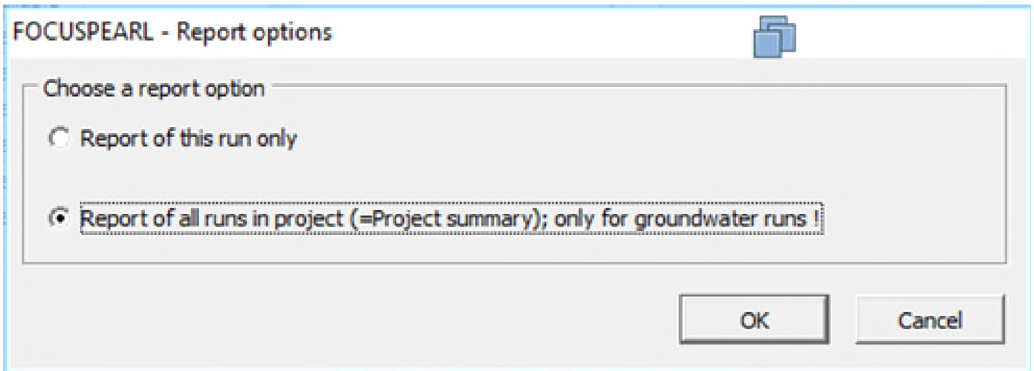
Figure 13: FOCUS PEARL 5.5.5: Run options



4.1.7 Viewing the results

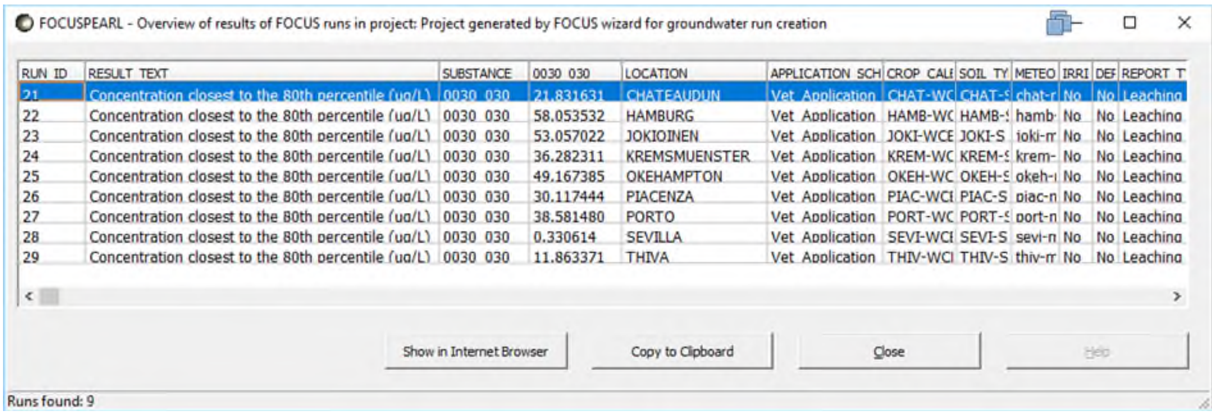
Now the results of the simulations can be evaluated. After a click at the “Report” button (see the “5” in Figure 1) two options are possible (see Figure 14): Report of a single run or a summary report of all runs in a project. Normally, the second option is sufficient since all information necessary for the risk assessment is presented.

Figure 14: FOCUS PEARL 5.5.5: Selecting type of report



In case the user selected "all runs in project" the form in Figure 15 is loaded. The percolate concentrations closeted to the 80th percentile (µg/L) is shown in the 4th column. In the 5th column the respective location is presented. The copy can be copied into other applications using the "copy to clipboard" button.

Figure 15: FOCUS PEARL 5.5.5: Summary report (percolate concentrations at 1 m soil depth)



RUN ID	RESULT TEXT	SUBSTANCE	0030 030	LOCATION	APPLICATION SCH	CROP CALE	SOIL TY	METEO	IRRI	DEF	REPORT T
21	Concentration closest to the 80th percentile (ug/L)	0030 030	21.831631	CHATEAUDUN	Vet Application	CHAT-WC	CHAT-S	chat-r	No	No	Leaching
22	Concentration closest to the 80th percentile (ug/L)	0030 030	58.053532	HAMBURG	Vet Application	HAMB-WC	HAMB-S	hamb-	No	No	Leaching
23	Concentration closest to the 80th percentile (ug/L)	0030 030	53.057022	JOKIOINEN	Vet Application	JOKI-WCE	JOKI-S	joki-m	No	No	Leaching
24	Concentration closest to the 80th percentile (ug/L)	0030 030	36.282311	KREMSMUENSTER	Vet Application	KREM-WC	KREM-S	krem-	No	No	Leaching
25	Concentration closest to the 80th percentile (ug/L)	0030 030	49.167385	OKEHAMPTON	Vet Application	OKEH-WC	OKEH-S	okeh-	No	No	Leaching
26	Concentration closest to the 80th percentile (ug/L)	0030 030	30.117444	PIACENZA	Vet Application	PIAC-WCI	PIAC-S	piac-n	No	No	Leaching
27	Concentration closest to the 80th percentile (ug/L)	0030 030	38.581480	PORTO	Vet Application	PORT-WC	PORT-S	port-n	No	No	Leaching
28	Concentration closest to the 80th percentile (ug/L)	0030 030	0.330614	SEVILLA	Vet Application	SEVI-WCI	SEVI-S	sevi-n	No	No	Leaching
29	Concentration closest to the 80th percentile (ug/L)	0030 030	11.863371	THIVA	Vet Application	THIV-WCI	THIV-S	thiv-m	No	No	Leaching

4.2 Surface water simulations

As already described in previous chapters, the FOCUS scenarios were originally developed for pesticides. This is the reason why the shell and some of the input parameters including default values are not in line with the needs in the risk assessment for veterinary compounds.

Several software tools belong to FOCUS SW. FOCUS SWASH is a shell which helps the user doing calculations in MACRO (calculating input from drainage systems), PRZM (calculating input via surface runoff and soil erosion) and TOXSWA (calculating surface water concentrations based on MACRO and PRZM data). As often additional risk mitigations are essential before pesticides can be registered the effect of respective measures (e.g., vegetated buffer zones for run-off) can be simulated using the SWAN model which can be also obtained via the FOCUS website.

In this manual the differences to the pesticide input parameters settings are explained and how successful simulations can be performed for veterinary compounds.

4.2.1 Downloading the software packages

The software package SWASH can be downloaded from the FOCUS website which is currently hosted by JRC. The current link to the FOCUS surface water models is

https://esdac.jrc.ec.europa.eu/projects/surface-water

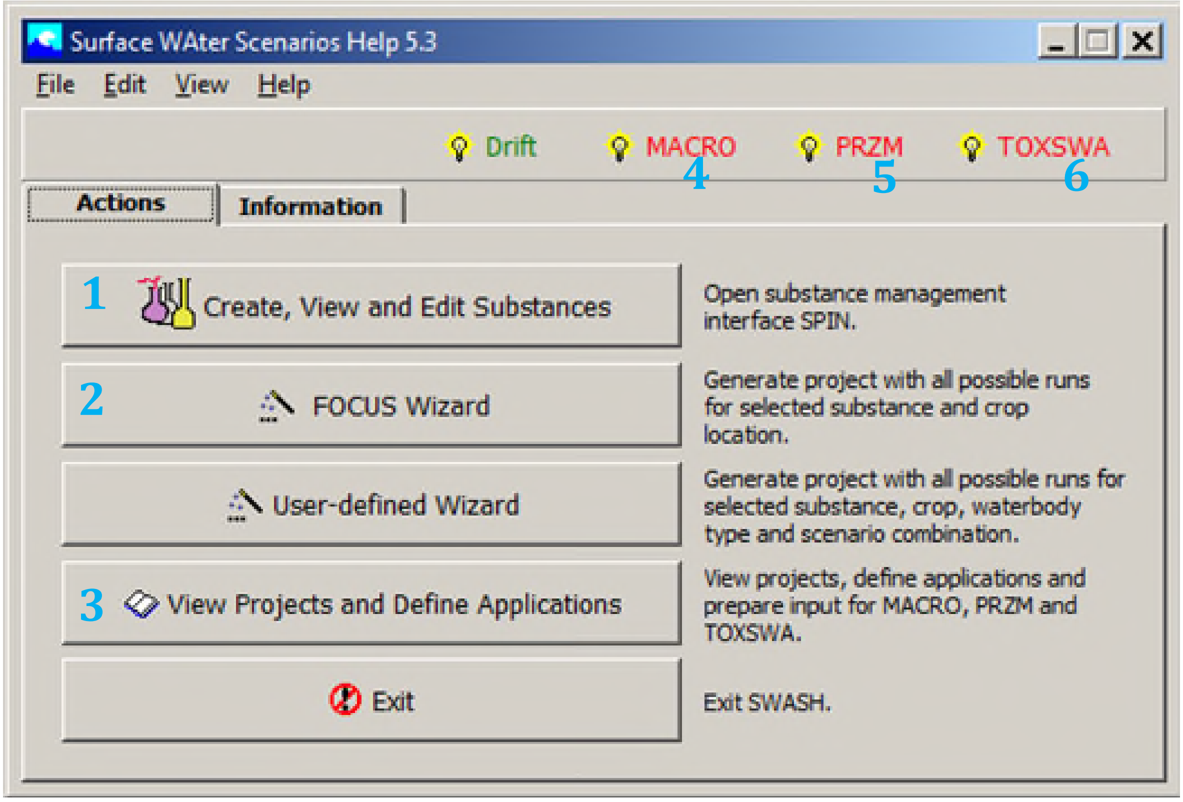
Please consider that you need to install SWASH before TOXSWA and PRZM.

- The default directory for TOXSWA is C:\SWASH\TOXSWA. In case you selected another drive than C for SWASH, the TOXSWA application should also be installed on that drive on subdirectory of the SWASH directory. For example, if you have installed SWASH on D:\SWASH then TOXSWA should be installed at: D:\SWASH\TOXSWA.
- The default directory for PRZM is C:\SWASH\PRZM. In case you selected another drive than C for SWASH, the PRZM application should also be installed on that drive on subdirectory of the SWASH directory. For example, if you have installed SWASH on D:\SWASH then PRZM should be installed at D:\SWASH\PRZM.

The separate tool SWAN can be obtained from the FOCUS website, too (same link as above for SWASH). Please consider that SWAN 5.0.1 was tested on 64-bit editions of Windows 7 and Windows 10. 32bit operating systems should be compatible but have not been tested. General Principles

After clicking at the FOCUS SWASH icon, a shell is loaded which helps the user through the process of editing input parameters and performing a sequence of three different models (see Figure 16). It is important to realise that in order to run simulations a fixed sequence has to be followed which is explained further below. The numbers in this figure refer to the different steps.

Figure 16: FOCUS SWASH

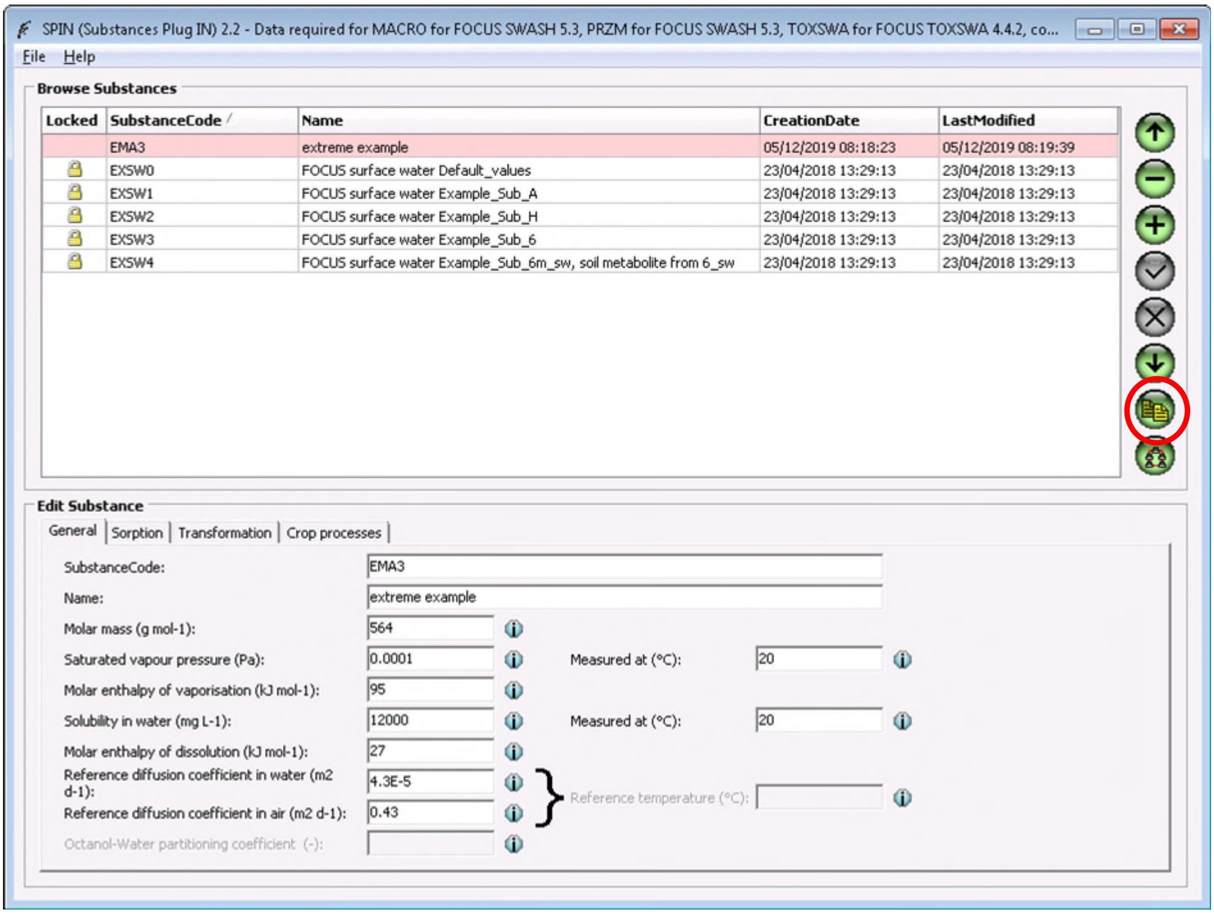


1. Enter substance specific parameters (e.g., sorption, degradation data)
2. Define the project (e.g., which compound and which crop should be included in the assessment)
3. Enter application data (e.g., application rate, incorporation depth, application window)
4. Run MACRO (model for the input from drainage systems)
5. Run PRZM (model for the input from run-off/erosion after heavy rainfall events)
6. Run TOXSWA (model for calculating concentrations in surface water bodies)

4.2.2 Editing substance input parameters

In the first step the substance parameters should be entered. The form in Figure 17 opens after clicking at the button (see the "1" in Figure 16). It is basically the same as in FOCUS PEARL (see, e.g., Figure 2). Background is that both models use the same database SPIN for pesticide input parameters. That means if a substance has been defined already when running FOCUS PEARL the dataset should already exist. Therefore, some information (e.g., name, molar mass, water solubility, crop parameters like TSCF) does not need to be entered again. However, a simulation with the FOCUS SWASH package needs more input parameters than FOCUS PEARL. Therefore, it is always necessary to go through the substance input parameter forms.

Figure 17: FOCUS SWASH: Editing general substance parameters



Next you should copy one of the default substances (e.g., “EXSW0”) using the copy button (see the red circle in Figure 17). This has an advantage compared to creating a new substance since most of the default values are already correctly set.

In the tab “General” enter the substance code and the name

Now, enter the values for following parameters:

- Molar mass
- Vapour pressure
- Water solubility

The remaining fields are set with correct default values.

Now, enter the sorption parameters in the tab “Sorption” or (see Figure 18). Dependent on the SPIN version the tab is also called “equilibrium sorption”. However, only

- Kom
- Freundlich sorption coefficient

have to be filled. The remaining fields are set with correct default values. However, these parameters have to be set three times in the sub-tabs Soil, Surface water and Sediment. As in most of the situations there are no specific Kom values for sediment/suspended sediment available the same information should be entered in all respective Kom-fields.

Figure 18: FOCUS SWASH: Editing sorption parameters (compartment soil)

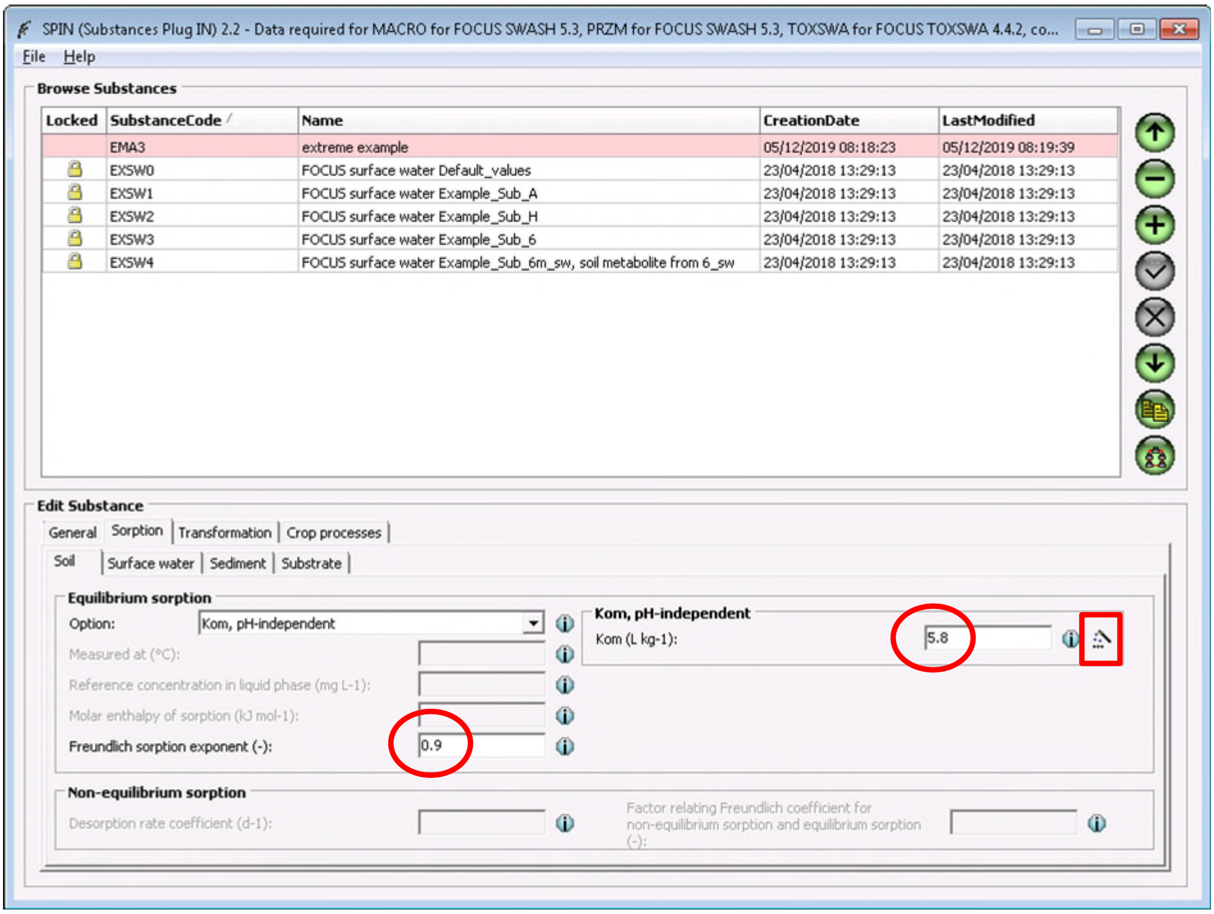


Figure 19 and Figure 20 show the sub-tabs for surface water and sediment, respectively.

Figure 19: FOCUS SWASH: Editing sorption parameters (compartment surface water)

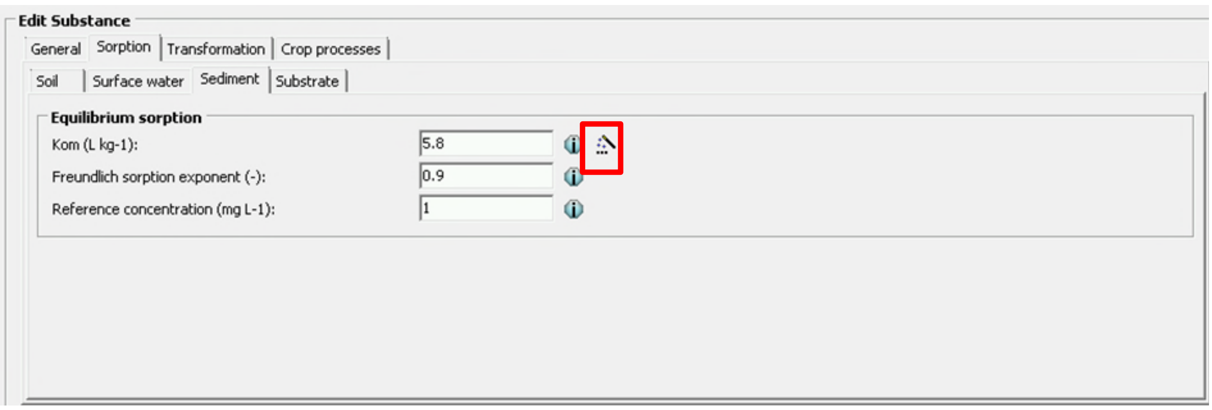
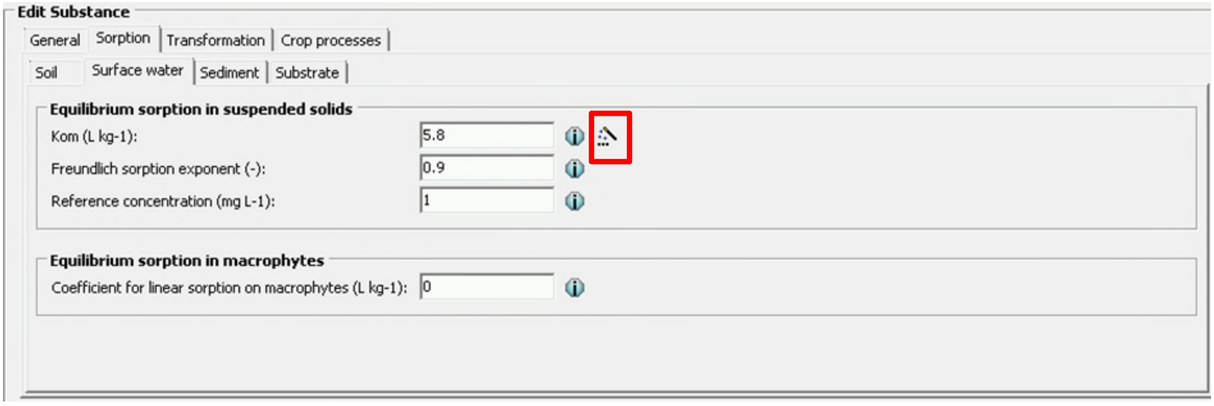


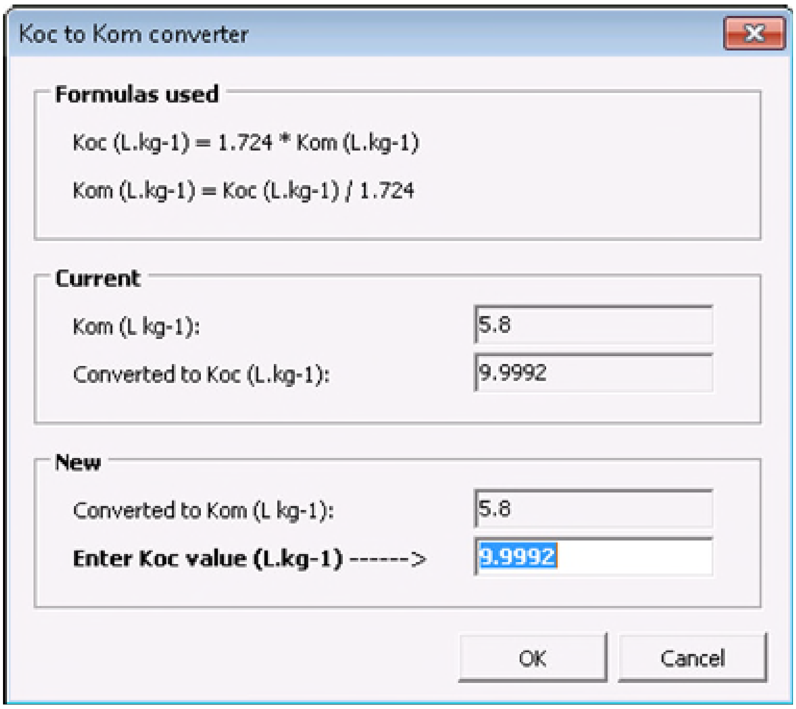
Figure 20: FOCUS SWASH: Editing sorption parameters (compartment sediment)



There is no need to enter any data in the sub-tab “Substrate”.

If information on the Kom is not available it can be calculated using the Koc after clicking at the wizard symbol (see the red rectangle). Then, the form in Figure 21 will appear.

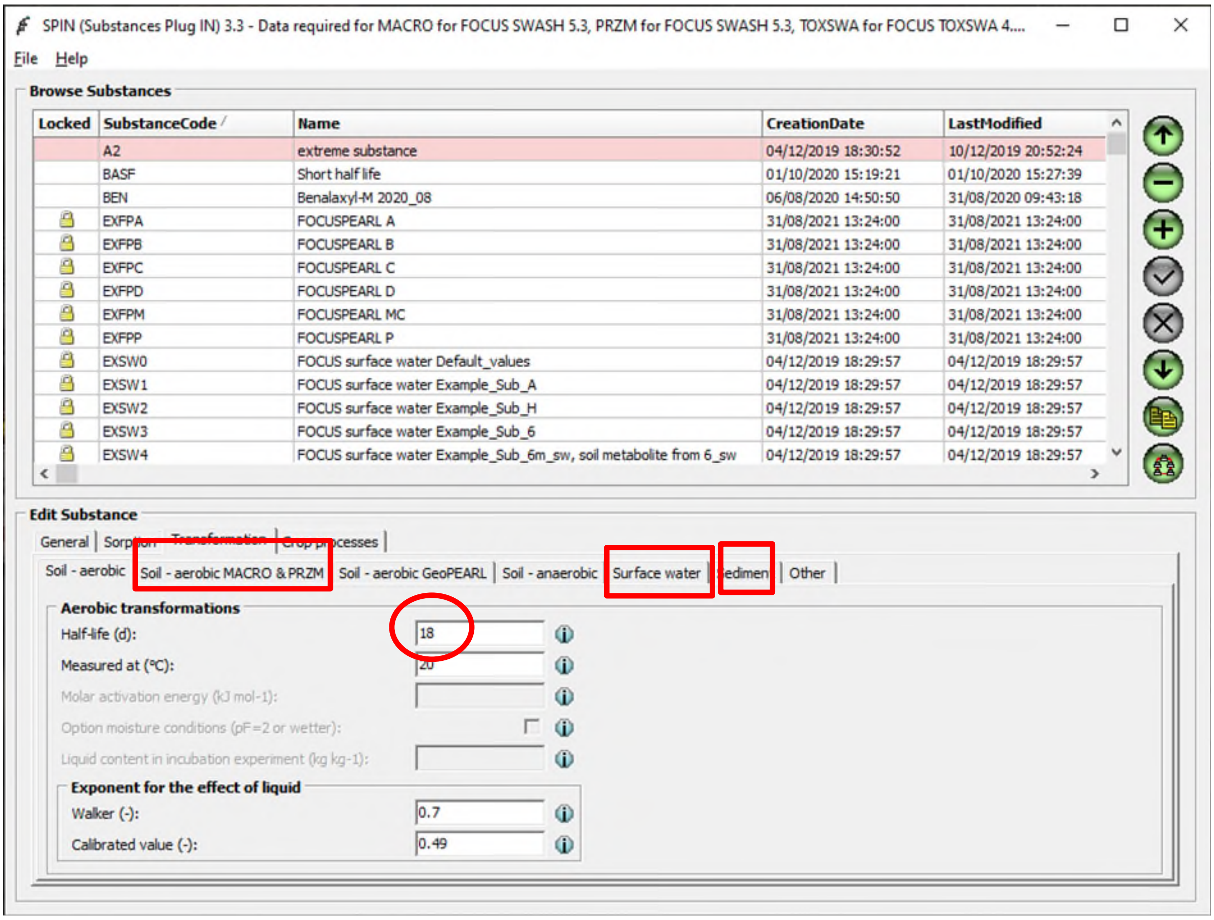
Figure 21: FOCUS SWASH: Calculating the Kom



In the next step, the degradation parameters have to be entered in the tab “Transformation” (see Figure 22). In principle, only a single field, the half-life at 20 °C, has to be entered. However, again these parameters have to be set in three sub-tabs

- “Soil – aerobic MACRO & PRZM” or “Soil-aerobic”,
- „Surface water“ and
- „Sediment“.

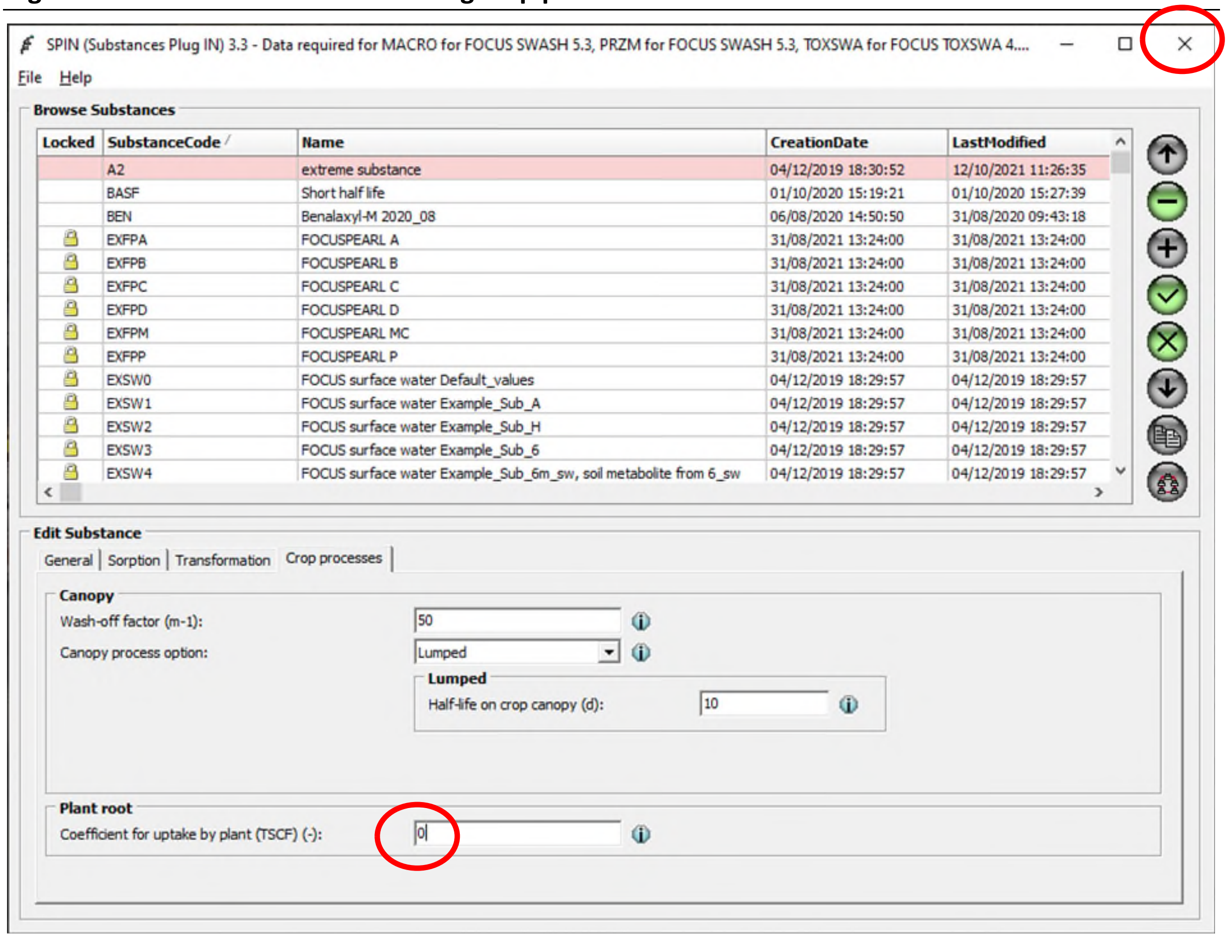
Figure 22: FOCUS SWASH: Editing degradation parameters



In the sub-tab "Soil – aerobic MACRO & PRZM" enter the DegT50 determined in the degradation study. In the sub-tab "Surface water" and "Sediment" results of water sediment studies can be considered. These studies are often not performed for veterinary compounds. Then, simply set the DegT50 in these compartments to 1000 d. There is no need to enter any data in the other sub-tabs. All other parameters in Figure 22 are set with correct default values. The Walker exponent describes the moisture dependency of the DegT50 and should not be changed.

Now, the crop parameters have to be entered in the tab "Crop processes" (see Figure 23). Again, only a single field, "the coefficient for uptake by plants", is relevant. It is important that this parameter is set to "0" by default. Unfortunately, the SWASH model uses a default of 0.5 here, which is common value for pesticides.

Figure 23: FOCUS SWASH: Editing crop parameters

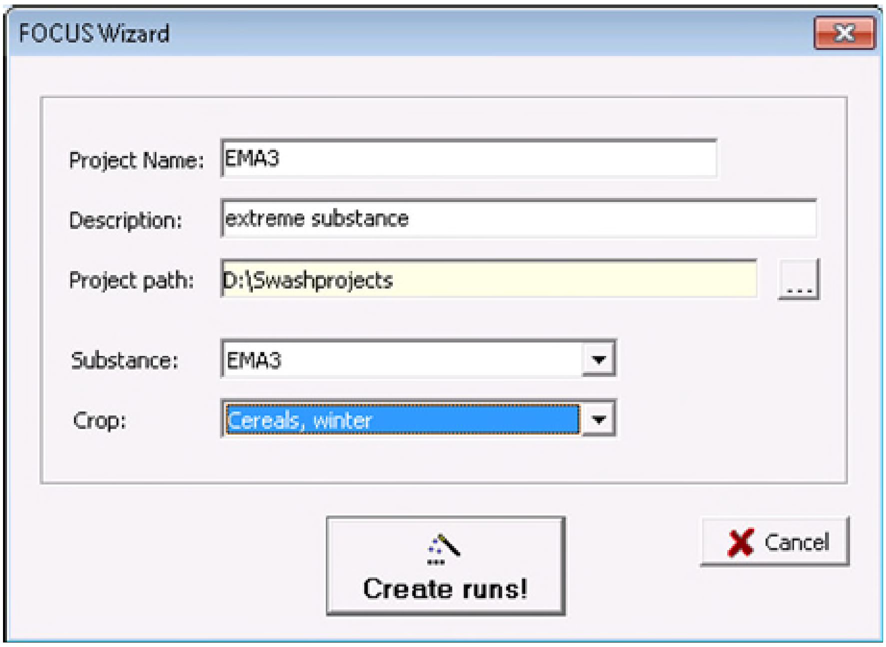


When all these substances specific input values have been entered, the form can be closed using the x-button in the top right corner of the form. The input fields referring to canopy processes are not relevant since the compound is incorporated before the crop is emerged.

4.2.3 Defining the project

In the next step the project has to be defined. The form in Figure 24 opens after clicking at the button ”Wizard” (see the “2” in Figure 16).

Figure 24: FOCUS SWASH: Defining the project

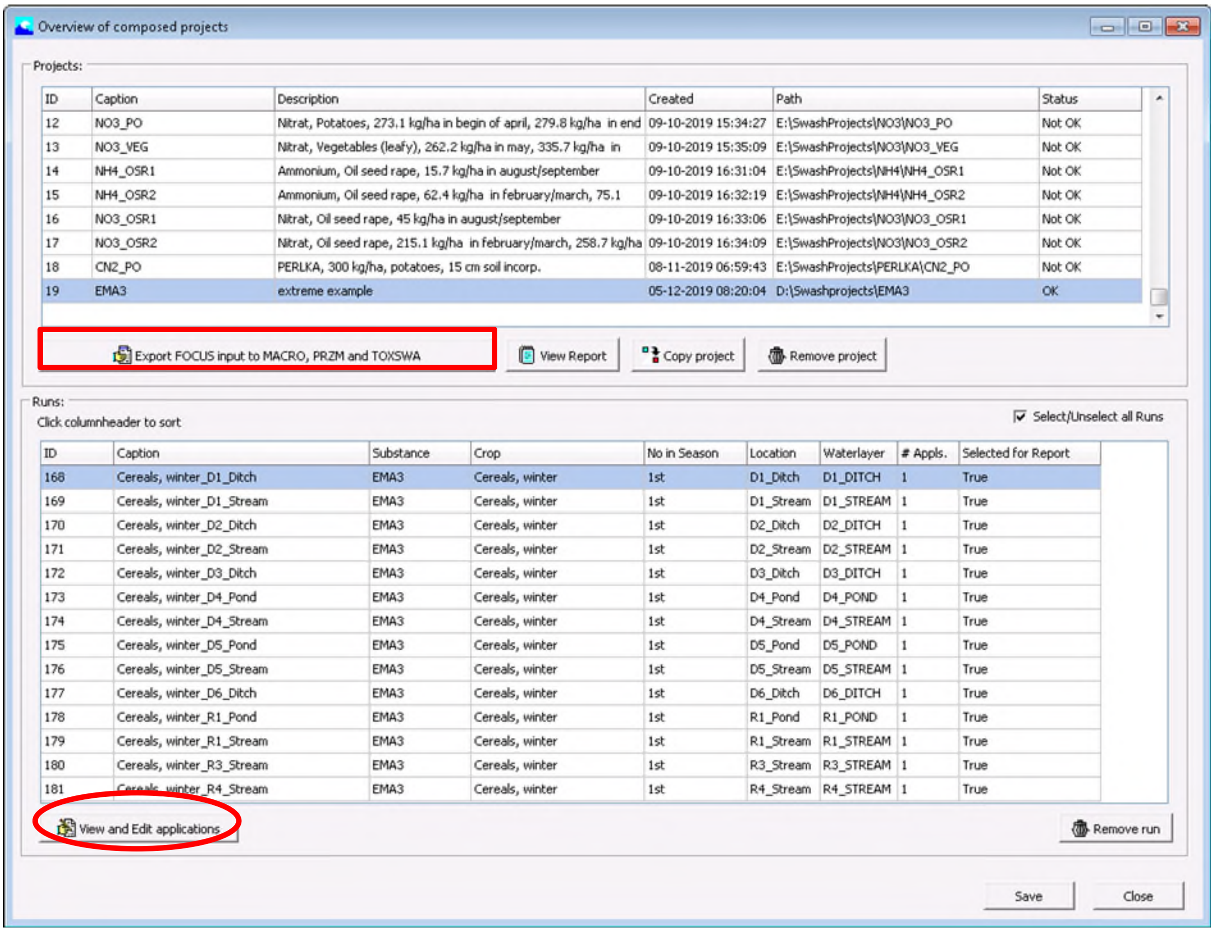


In this form a name and a description for the project have to be defined. Then, there are two more fields for the substance and the crop (normally: winter cereals) that has to be chosen. There is normally no need to change the project path. After having clicked at "Create runs" the project will be created.

4.2.4 Editing application input parameters

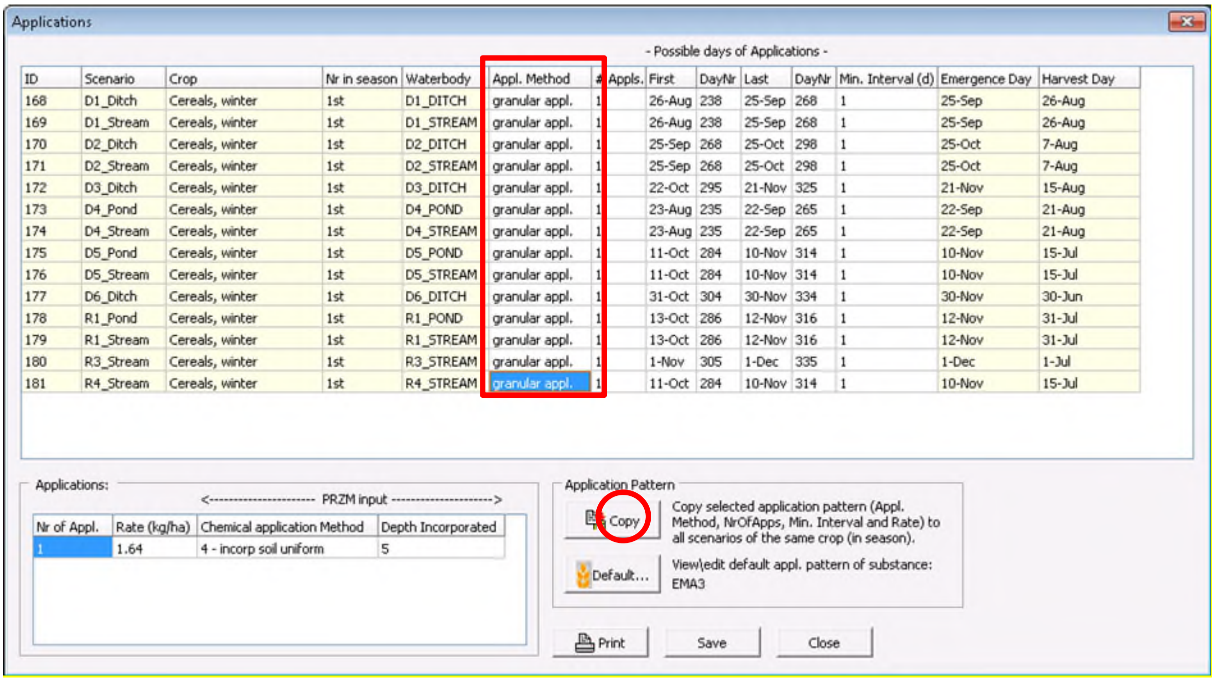
In the next step the application parameters must be entered. The form in Figure 25 with a list of all projects opens after clicking at the button (see the "3" in Figure 16).

Figure 25: FOCUS SWASH: Viewing projects



In order to edit the application data, click at the respective button in Figure 25 (red circle). That will load a form where the application pattern of the selected project can be entered.

Figure 26: FOCUS SWASH: Editing application parameters



ID	Scenario	Crop	Nr in season	Waterbody	Appl. Method	# Appls.	First	DayNr	Last	DayNr	Min. Interval (d)	Emergence Day	Harvest Day
168	D1_Ditch	Cereals, winter	1st	D1_DITCH	granular appl.	1	26-Aug	238	25-Sep	268	1	25-Sep	26-Aug
169	D1_Stream	Cereals, winter	1st	D1_STREAM	granular appl.	1	26-Aug	238	25-Sep	268	1	25-Sep	26-Aug
170	D2_Ditch	Cereals, winter	1st	D2_DITCH	granular appl.	1	25-Sep	268	25-Oct	298	1	25-Oct	7-Aug
171	D2_Stream	Cereals, winter	1st	D2_STREAM	granular appl.	1	25-Sep	268	25-Oct	298	1	25-Oct	7-Aug
172	D3_Ditch	Cereals, winter	1st	D3_DITCH	granular appl.	1	22-Oct	295	21-Nov	325	1	21-Nov	15-Aug
173	D4_Pond	Cereals, winter	1st	D4_POND	granular appl.	1	23-Aug	235	22-Sep	265	1	22-Sep	21-Aug
174	D4_Stream	Cereals, winter	1st	D4_STREAM	granular appl.	1	23-Aug	235	22-Sep	265	1	22-Sep	21-Aug
175	D5_Pond	Cereals, winter	1st	D5_POND	granular appl.	1	11-Oct	284	10-Nov	314	1	10-Nov	15-Jul
176	D5_Stream	Cereals, winter	1st	D5_STREAM	granular appl.	1	11-Oct	284	10-Nov	314	1	10-Nov	15-Jul
177	D6_Ditch	Cereals, winter	1st	D6_DITCH	granular appl.	1	31-Oct	304	30-Nov	334	1	30-Nov	30-Jun
178	R1_Pond	Cereals, winter	1st	R1_POND	granular appl.	1	13-Oct	286	12-Nov	316	1	12-Nov	31-Jul
179	R1_Stream	Cereals, winter	1st	R1_STREAM	granular appl.	1	13-Oct	286	12-Nov	316	1	12-Nov	31-Jul
180	R3_Stream	Cereals, winter	1st	R3_STREAM	granular appl.	1	1-Nov	305	1-Dec	335	1	1-Dec	1-Jul
181	R4_Stream	Cereals, winter	1st	R4_STREAM	granular appl.	1	11-Oct	284	10-Nov	314	1	10-Nov	15-Jul

Nr of Appl.	Rate (kg/ha)	Chemical application Method	Depth Incorporated
1	1.64	4 - incorp soil uniform	5

First, enter "granular application" for every run in the project (see the red rectangle in Figure 26). Do it manually and do not use the copy button because of a bug in the SWASH shell. The application method (e.g., granular application vs. incorporation) is very sensitive for the D-scenarios.

Then select one of the R-scenarios (e.g., R4_stream as in Figure 26) and edit the fields under "Applications" in the bottom left part of the form:

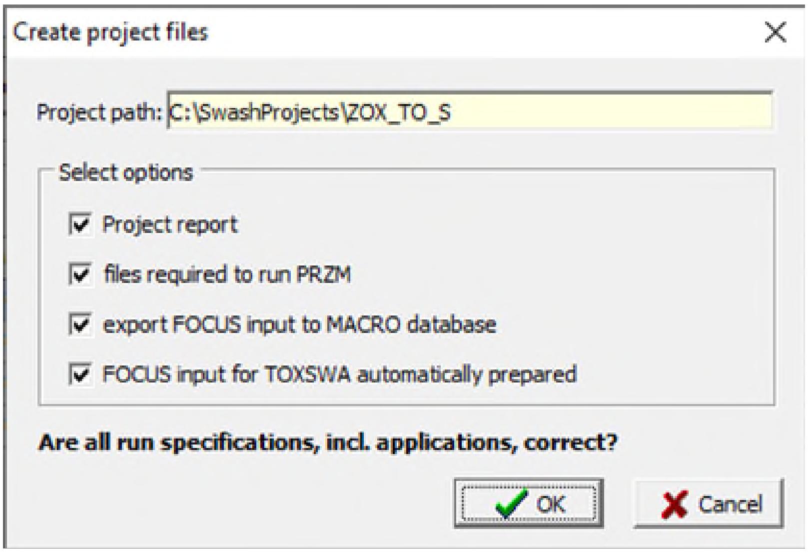
- Rate (kg/ha): The individual application rate of the compound
- Chemical application model: 4 – incorporation soil uniform
- Depth Incorporated: 5 cm (for annual crops)

Here, you can use the copy button (red circle) to put the information into all scenarios.

Then, all information about the application has been given and the form should be closed using the close button.

At this point, all input parameters have been entered in the SWASH shell and all information has to be forwarded to the three simulation models. Therefore, the button "Export FOCUS input to MACRO, PRZM and TOXSWA" has to be used (see the red rectangle in Figure 25). That will load a form (see Figure 27) where all default values can be simply accepted by clicking at the OK-button. In the next step the simulation models should be opened for the further procedure. In case a substance record has been created previously in PEARL without editing the additional input parameters for the FOCUS SW models a warning will be displayed. The user should then return to the SPIN database and enter the missing values.

Figure 27: FOCUS SWASH: Transferring input to the simulation models



4.2.5 Running MACRO

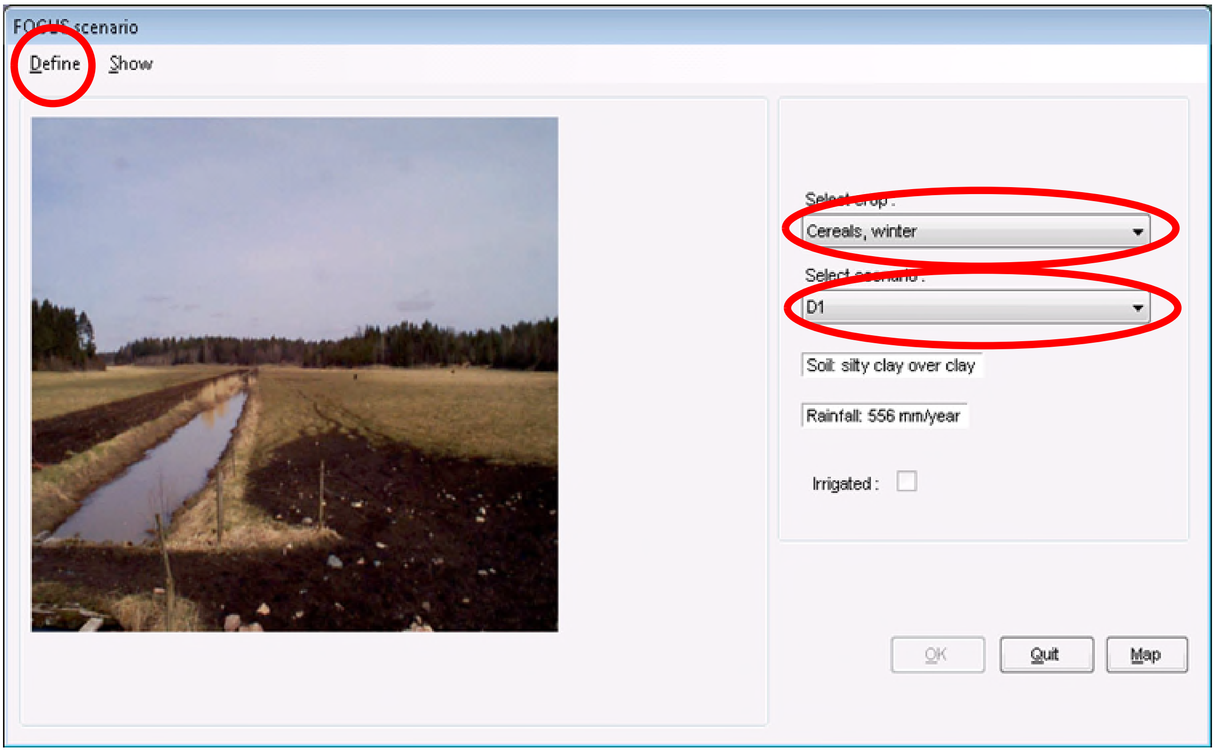
MARCO is loaded when the respective button (see the “4” in Figure 16) is used. The model is shown in Figure 28.

Figure 28: FOCUS MACRO: Main form

In order to prepare the MACRO simulation first click at "define scenario" and then pick "surface water". This will load the form presented in Figure 29 where the input parameter previously defined in the SWASH shell can be selected.

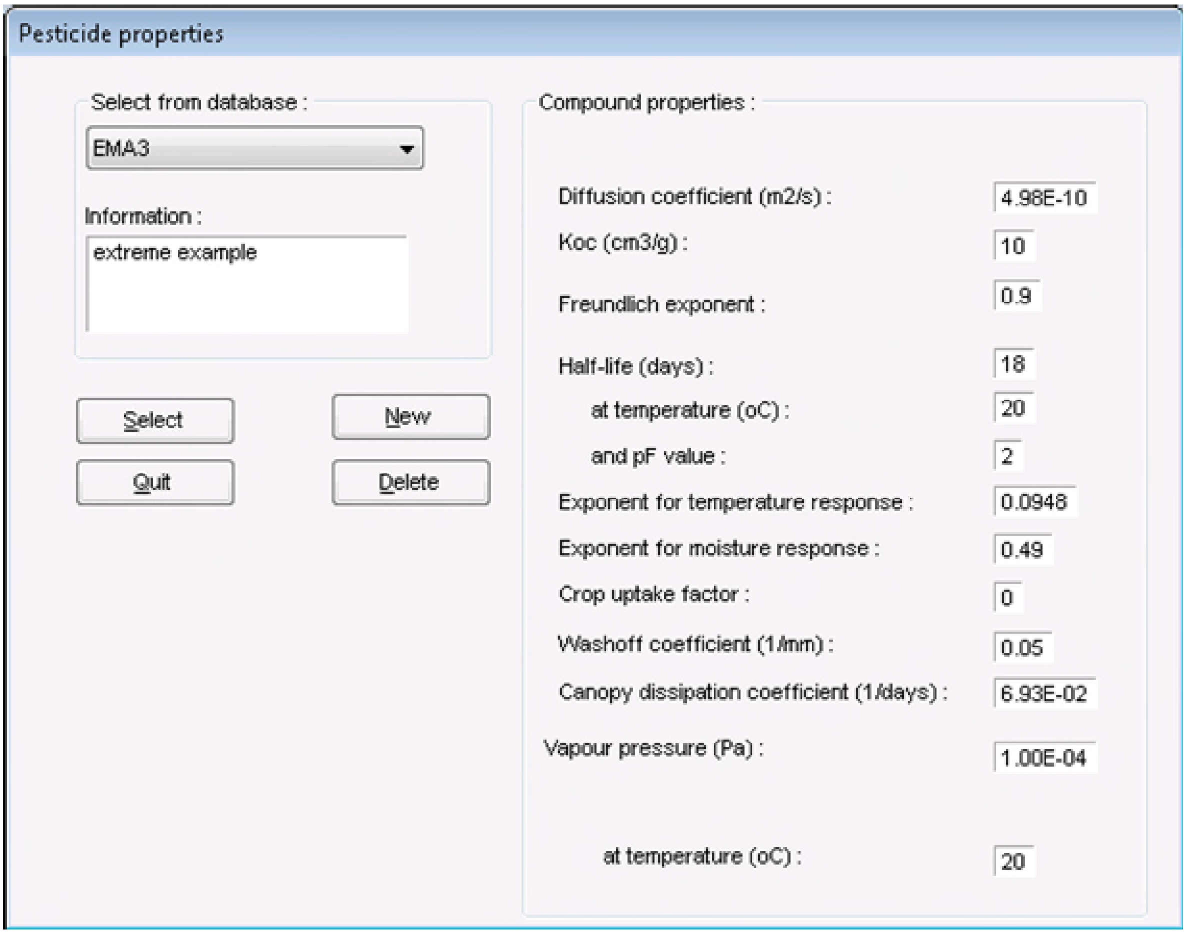
Here you have to set the crop (normally winter cereals) and one of the scenarios (e.g., D1). Unfortunately, the MACRO shell cannot handle multi-selections of D-scenarios. So, all D-scenarios have to be picked in a sequence. After having picked one of the D-scenarios, select the compound for the simulation (use the menu in the top, see the red cirlce in Figure 29). The fields for the soil type and the rainfall cannot be changed and are only informative.

Figure 29: FOCUS MACRO: Scenario form



Substance data can be selected by picking one of the substances in the list followed by a click at "Select". See the red circles in Figure 30. If all information has been correctly exported in the SWASH shell previously (see Figure 25 and Figure 27), your substance should be present in the list.

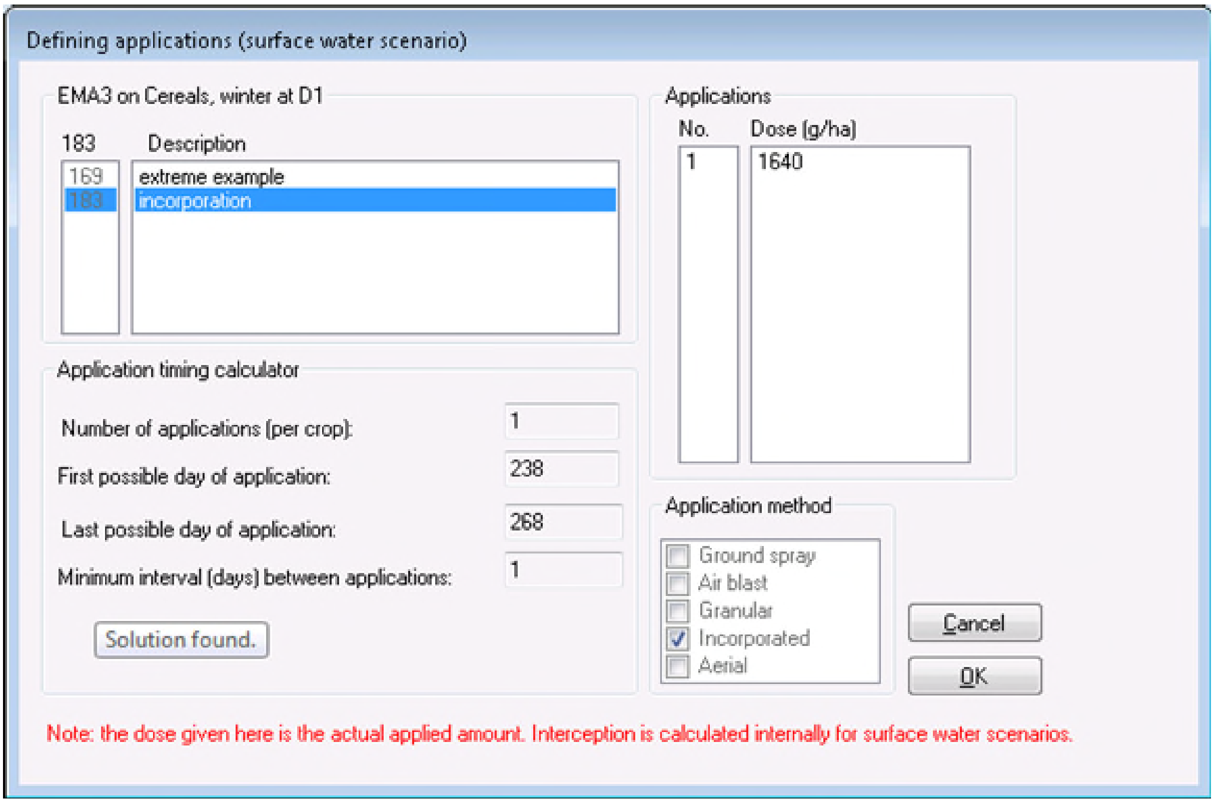
Figure 30: FOCUS MACRO: Selecting the substance



Then, select the relevant application pattern via "Define" followed by "application" in the menu (Figure 29). The procedure here is

1. Click at the suitable application pattern (i.e., name of the predefined project)
2. Click at OK

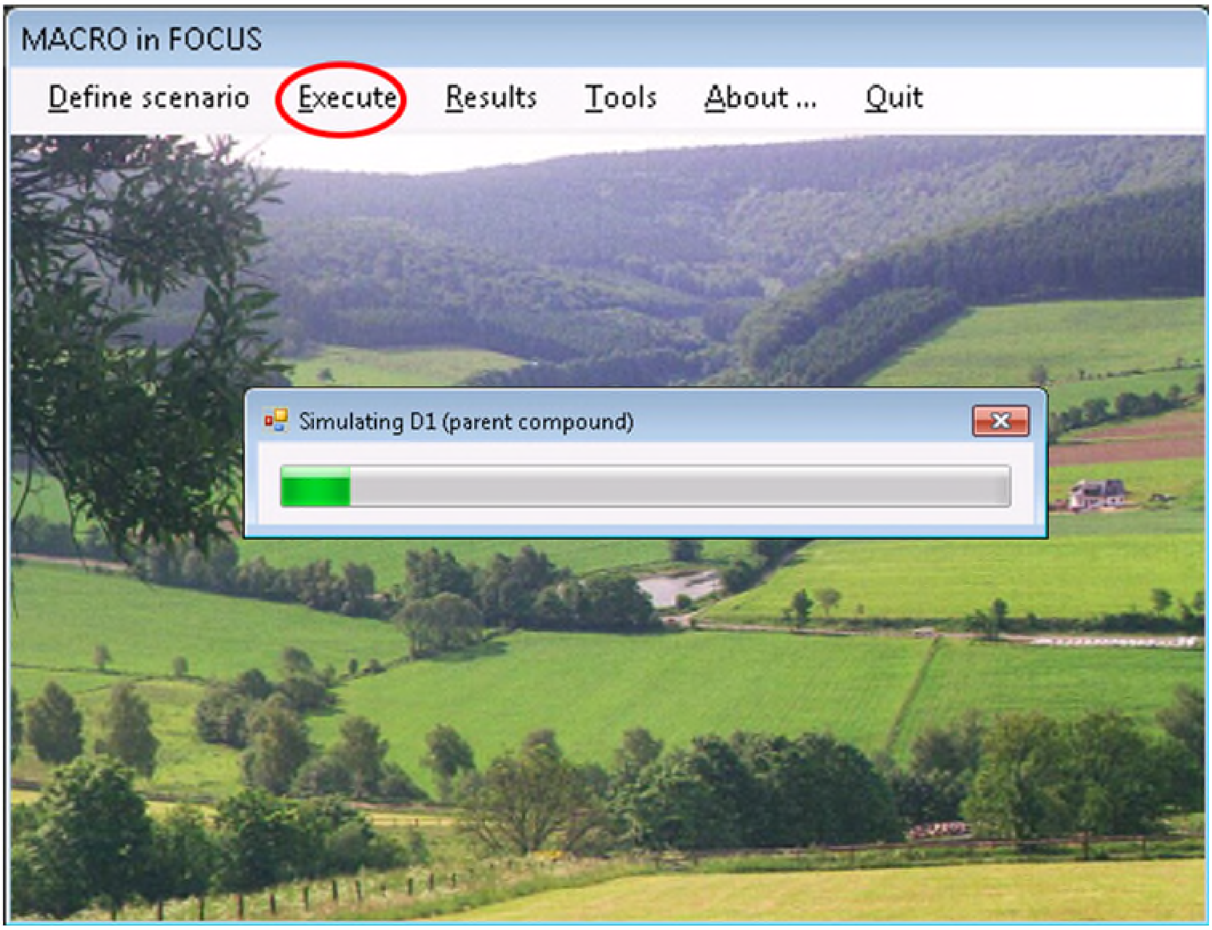
Figure 31: FOCUS MACRO: Selecting the application



All necessary information on this individual MACRO run has now been entered. The OK button should be enabled and the form can be closed using this button (see Figure 29).

Now, principally a simulation could be performed. Use the menu item “Execute” followed by “current” (see Figure 32).

Figure 32: FOCUS MACRO: Performing a single simulation

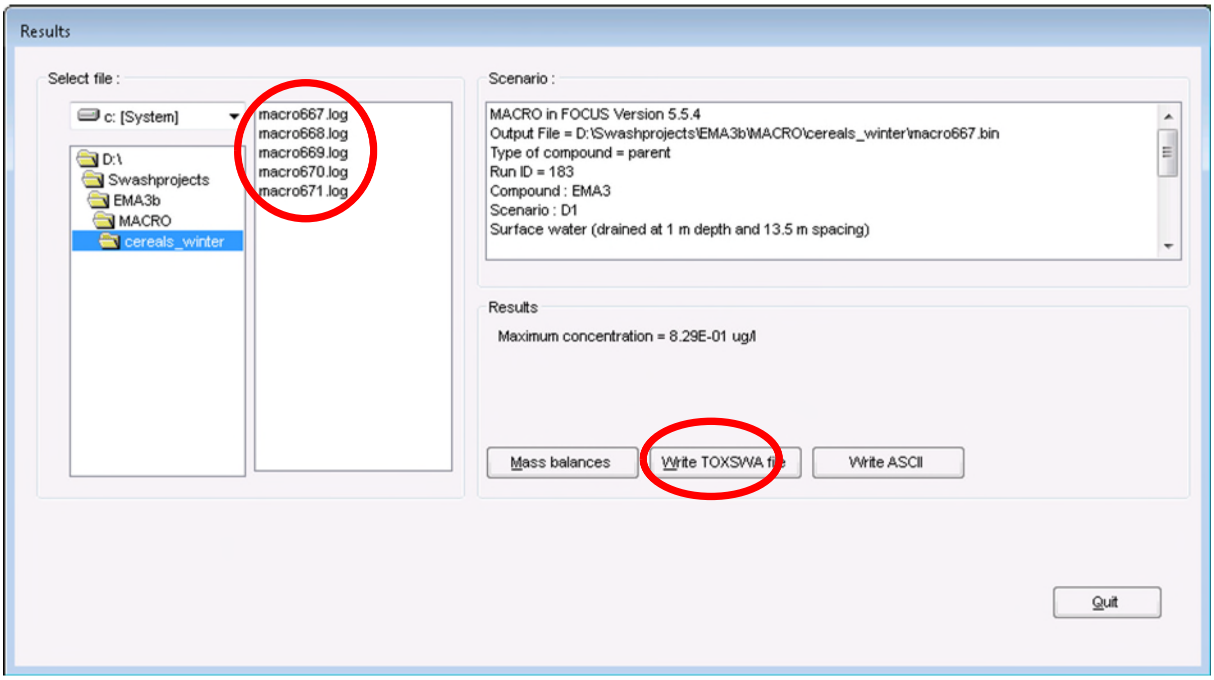


Alternatively, you could also add the simulation to a batch job. Please use the same menu item, but then pick “setup up batch file” and “add to batch”. The run will not directly start, instead you can define another scenario (e.g., D2) or a different project. Once, all runs have been defined “execute” followed by “Batch” will start all simulations in the queue.

When the simulations are done, the results have to be prepared in a way that TOXSWA is able to process the results. The menu item “Results” has to be used (see again Figure 32) for this purpose. The command will load the form presented in Figure 33. After every simulation a log file is created. Select a log file and then click at the button “write TOXSWA file”. The procedure has to be repeated for every MACRO run. After that has been done the form can be closed (button Quit).

Then, MACRO can be closed using the Quit button in Figure 32.

Figure 33: FOCUS MACRO: Creating TOXSWA input from MACRO

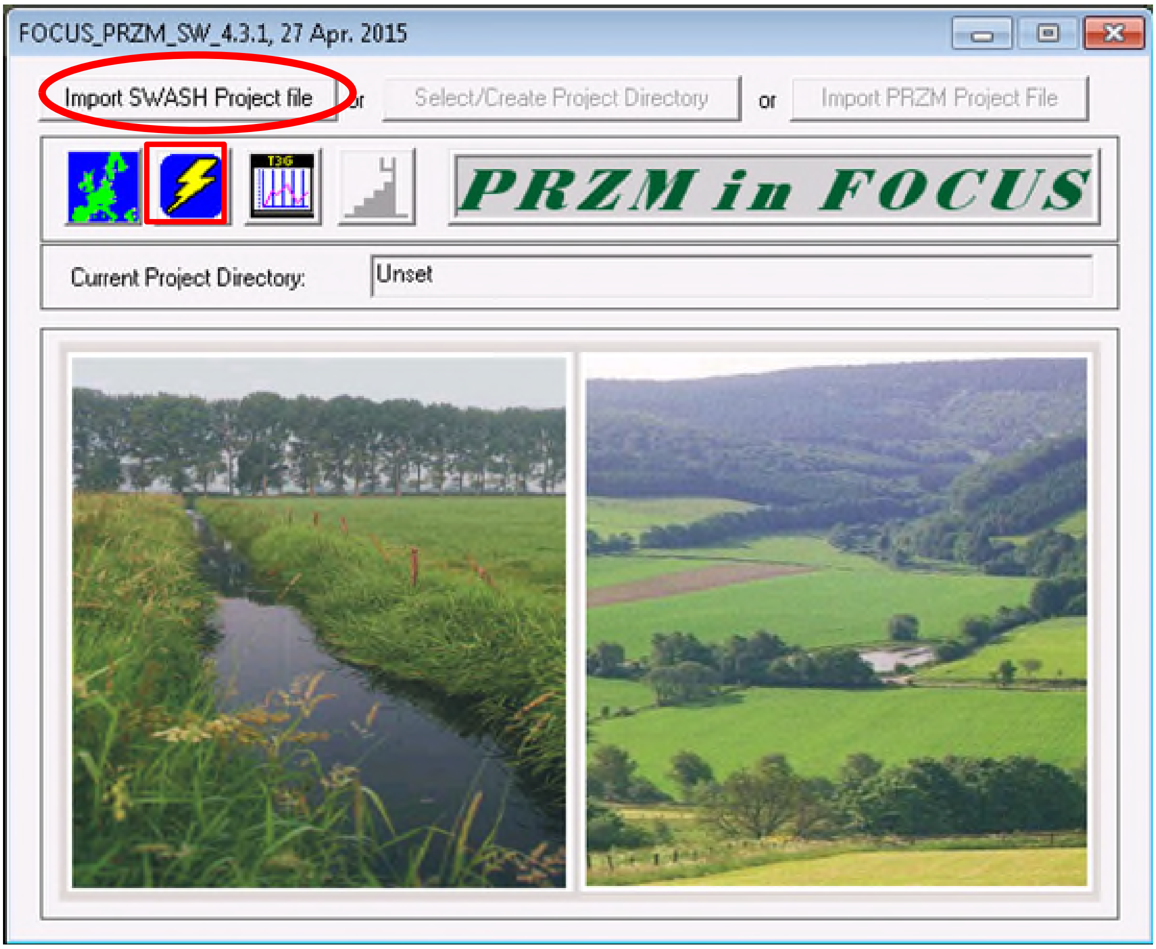


4.2.6 Running PRZM

PRZM is loaded when the respective button (see the “5” in Figure 16) is used. The model is shown in Figure 34.

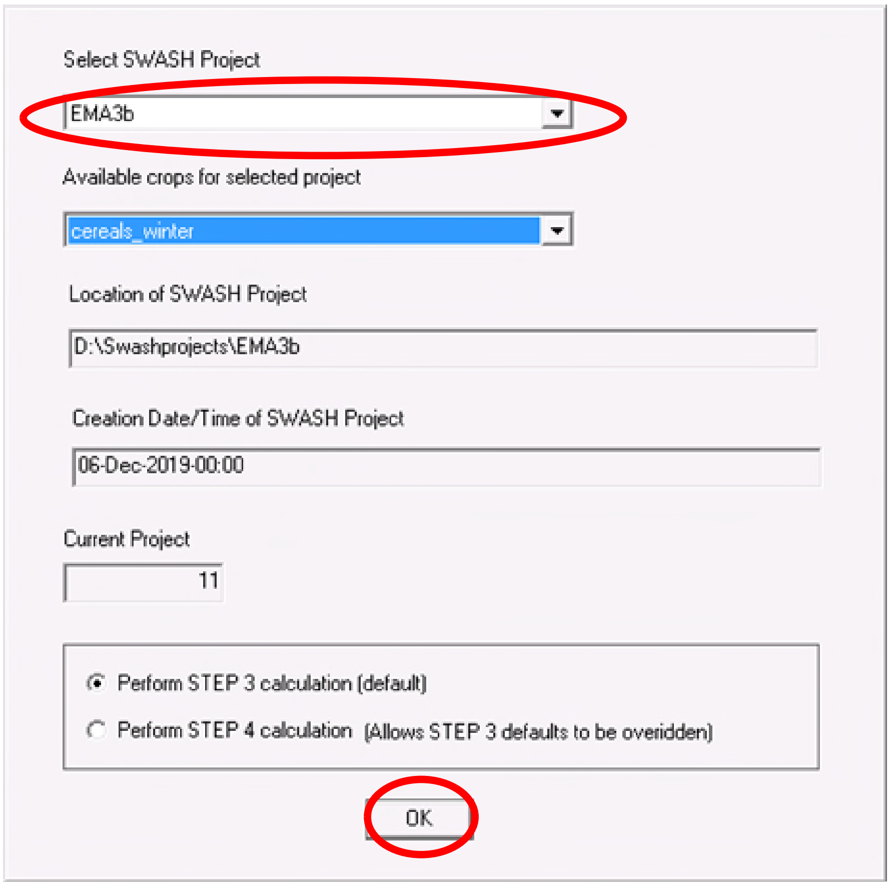
First, the information from SWASH has to be imported into this model using the button “Import SWASH Project file”.

Figure 34: PRZM: Main form



The button will open a new form where the previously defined SWASH project and the connected crop can be selected. Do not use the other options, instead click directly at OK to close the form.

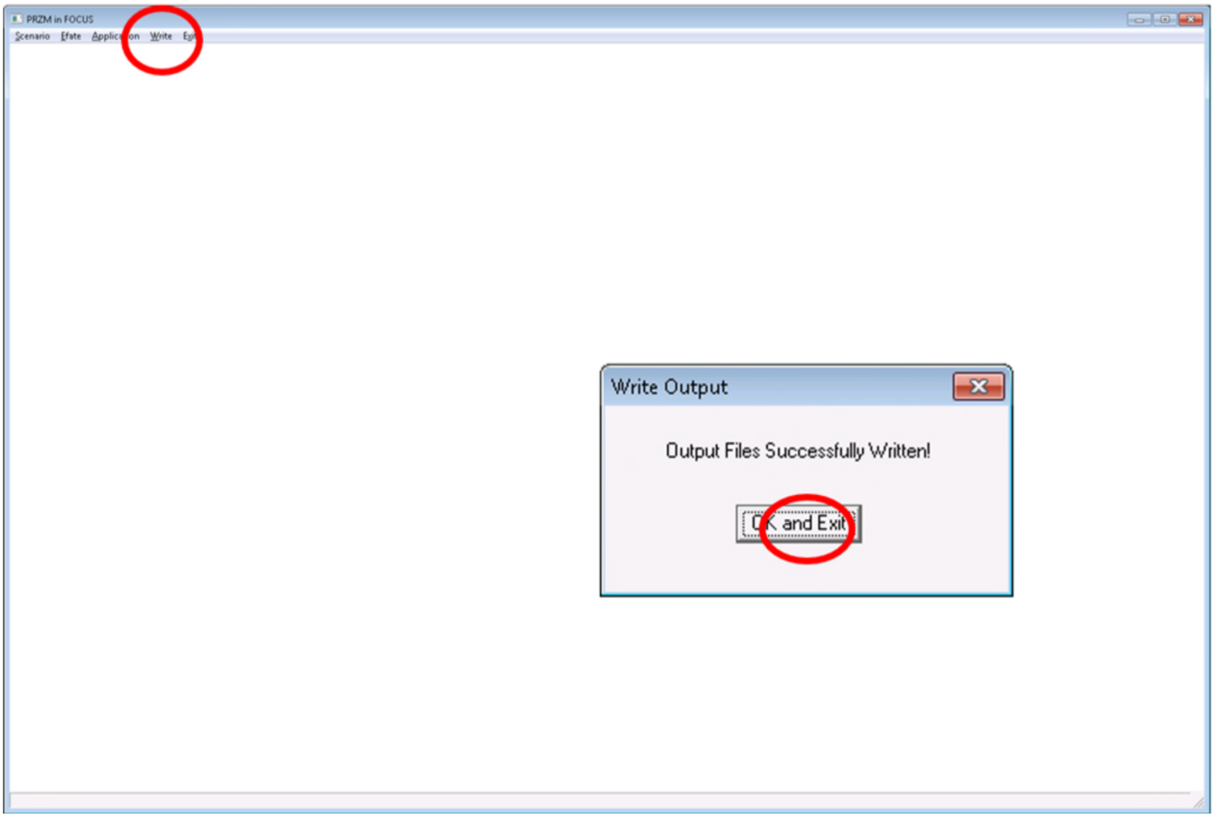
Figure 35: PRZM: Selecting a SWASH project



The button "OK" will directly open a second form (see Figure 35) which should be closed using the menu item "Write" followed by "OK and Exit". It is not necessary to do any editing here.

Now, all PRZM runs in the project can be performed by clicking at the lightning on the main PRZM form (see the red rectangle in Figure 34). After the simulation you can leave PRZM (use the "X" button in the top right corner of the form).

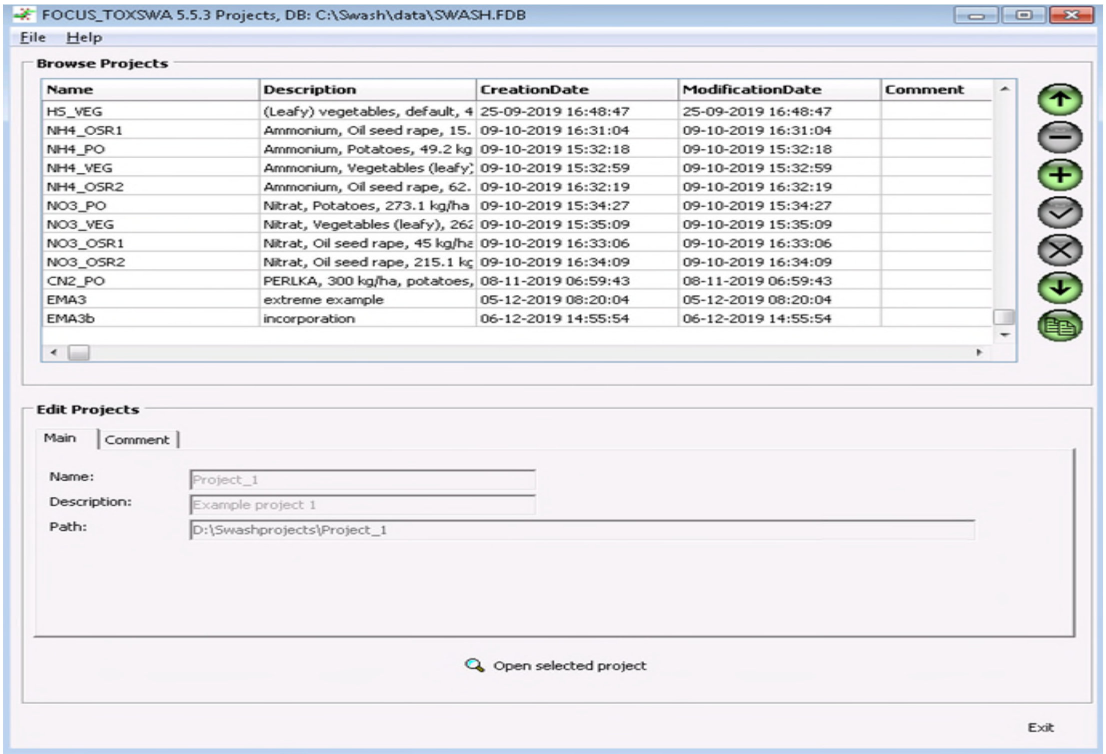
Figure 36: PRZM: Preparing input from SWASH for PRZM



4.2.7 Running TOXSWA

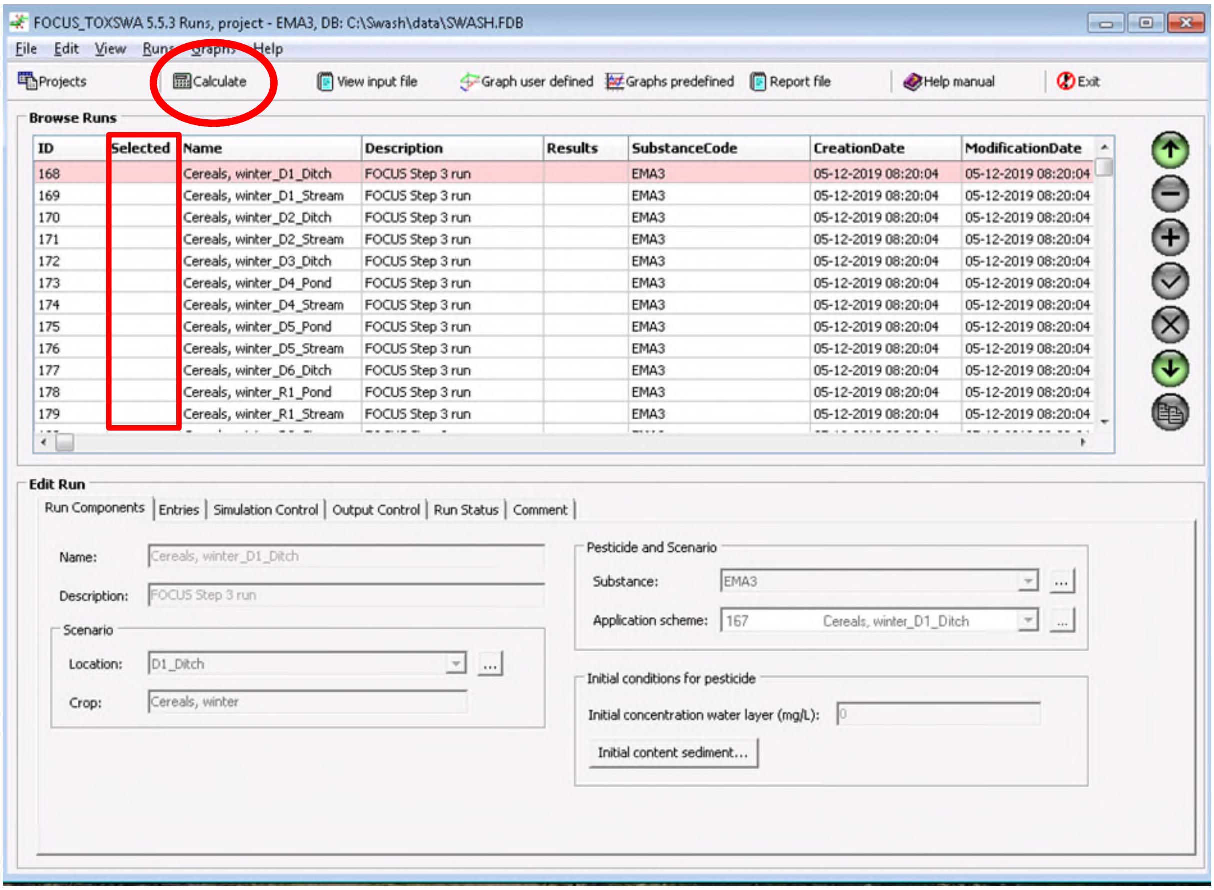
TOXSWA is loaded when the respective button (see the "6" in Figure 16) is used. The model always starts with the list of all projects which is shown in Figure 37. This is the same list as in the SWASH database. In order to perform a simulation a project must be picked (e.g. by double-clicking at the respective line in the table).

Figure 37: TOXSWA: List of all projects



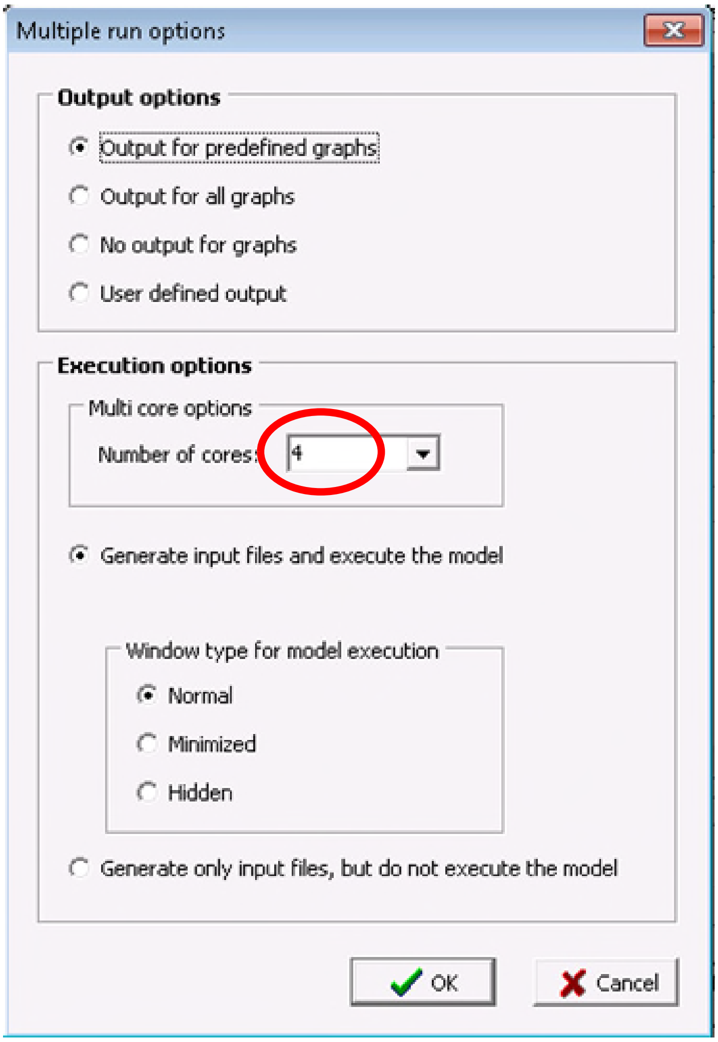
This will load a detailed list of all runs within the selected project as shown in Figure 38. From this form you can run TOXSWA (see the red circle) after the respective runs have been selected (see red rectangle).

Figure 38: TOXSWA: Project view



Before TOXSWA actually starts some further options have to be addressed as shown in Figure 39. Most relevant here is only the number of cores. Dependent on this value the number of parallel TOXSWA runs is set. Suitable setting here could reduce the time for doing the simulations significantly.

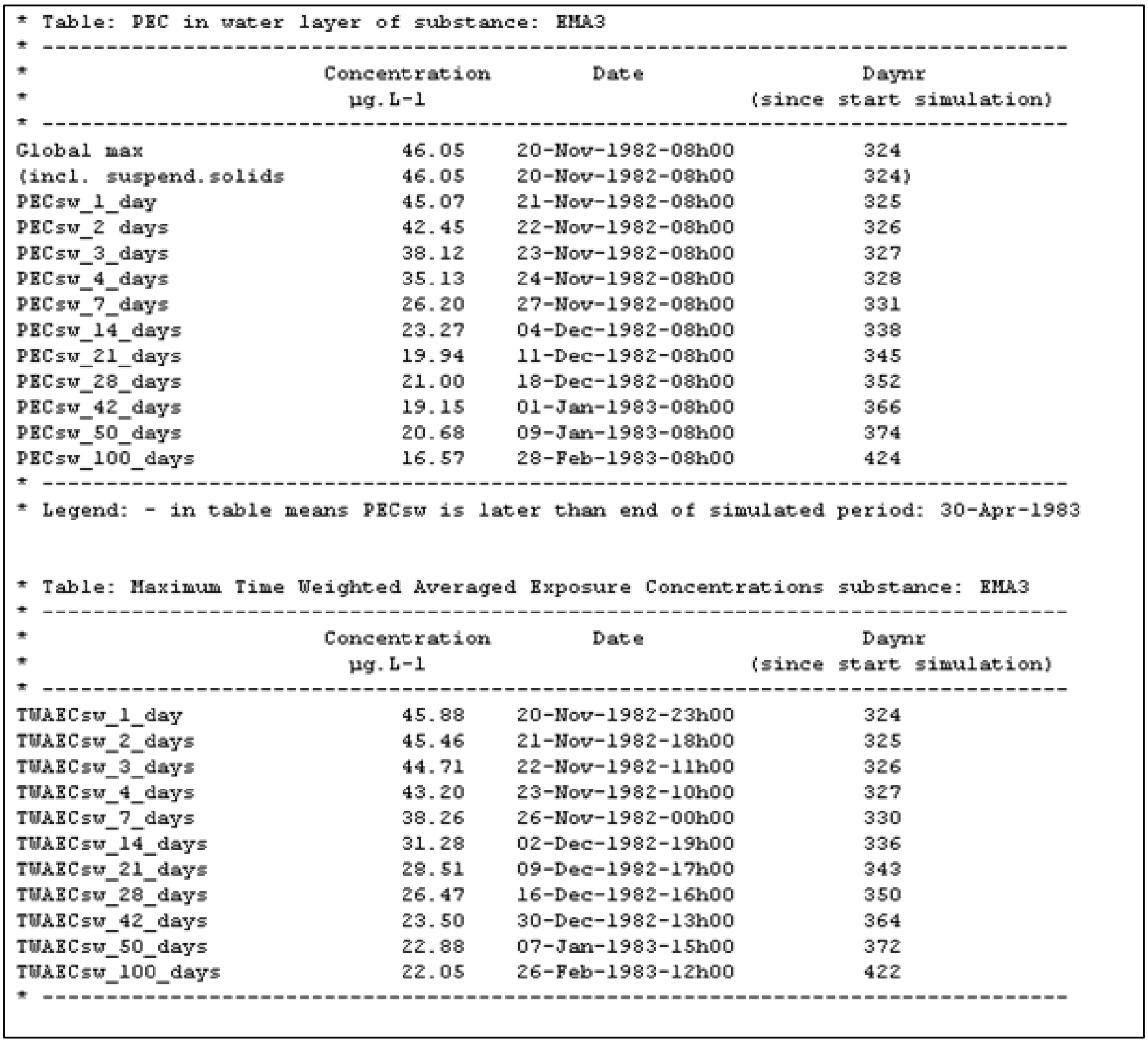
Figure 39: TOXSWA: Run options



After all runs have been performed the results can be evaluated. Select a simulation and then click at "Report file" in the menu bar (see Figure 38). The command will load the results (see Figure 40). Most relevant are the maximum concentrations in water values (PECmax in µg/L) over the simulation period of 1 year. Sometimes also the TWAs could be interesting. More information about using TWAs in the risk assessment can be found in question 17 of EMA (2005).

Unfortunately, TOXSWA does not present PECmax values for several runs within a list (like PEARL). However, according to the results of EFSA's repair action (EFSA 2020) it is expected that the updated models will run over 20 years so that an output format similar as PEARL (with an official percentile as endpoint) would be given.

Figure 40: TOXSWA: Cut-out of the report file



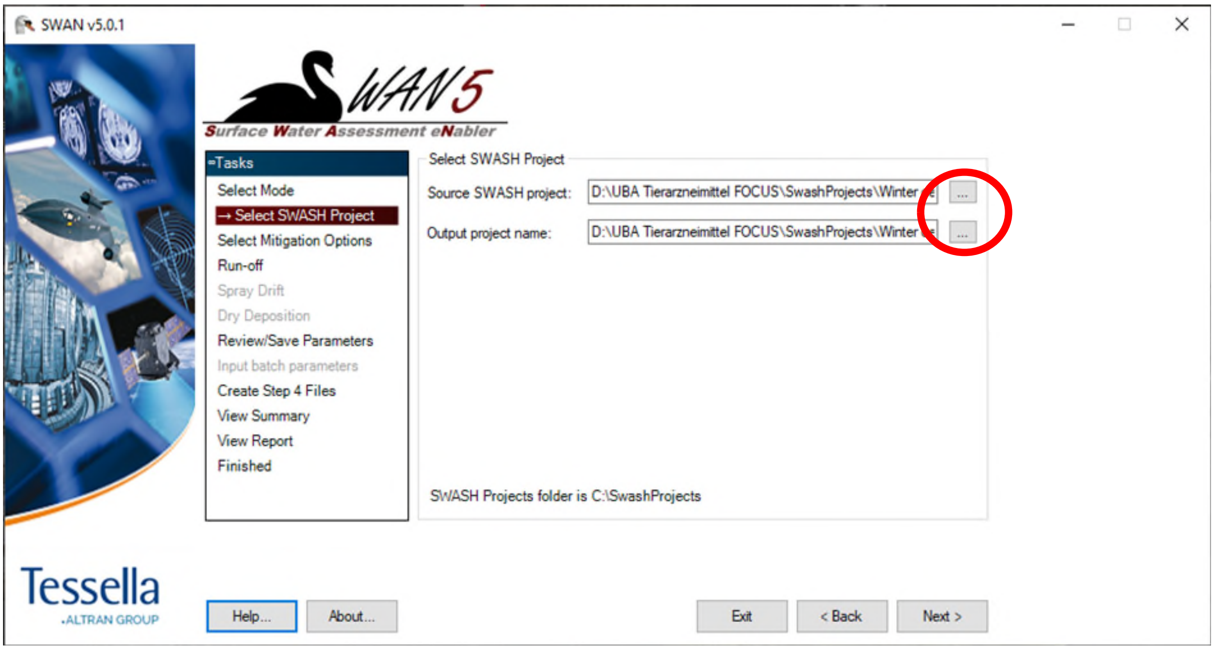
```
* Table: PEC in water layer of substance: EMA3
* ------------------------------------------------------------------------------
*                       Concentration        Date                Daynr
*                        µg.L-1                          (since start simulation)
* ------------------------------------------------------------------------------
Global max                   46.05     20-Nov-1982-08h00            324
(incl. suspend.solids        46.05     20-Nov-1982-08h00            324)
PECsw_1_day                  45.07     21-Nov-1982-08h00            325
PECsw_2 days                 42.45     22-Nov-1982-08h00            326
PECsw_3_days                 38.12     23-Nov-1982-08h00            327
PECsw_4_days                 35.13     24-Nov-1982-08h00            328
PECsw_7_days                 26.20     27-Nov-1982-08h00            331
PECsw_14_days                23.27     04-Dec-1982-08h00            338
PECsw_21_days                19.94     11-Dec-1982-08h00            345
PECsw_28_days                21.00     18-Dec-1982-08h00            352
PECsw_42_days                19.15     01-Jan-1983-08h00            366
PECsw_50_days                20.68     09-Jan-1983-08h00            374
PECsw_100_days               16.57     28-Feb-1983-08h00            424
* ------------------------------------------------------------------------------
* Legend: - in table means PECsw is later than end of simulated period: 30-Apr-1983


* Table: Maximum Time Weighted Averaged Exposure Concentrations substance: EMA3
* ------------------------------------------------------------------------------
*                       Concentration        Date                Daynr
*                        µg.L-1                          (since start simulation)
* ------------------------------------------------------------------------------
TWAECsw_1_day                45.88     20-Nov-1982-23h00            324
TWAECsw_2_days               45.46     21-Nov-1982-18h00            325
TWAECsw_3_days               44.71     22-Nov-1982-11h00            326
TWAECsw_4_days               43.20     23-Nov-1982-10h00            327
TWAECsw_7_days               38.26     26-Nov-1982-00h00            330
TWAECsw_14_days              31.28     02-Dec-1982-19h00            336
TWAECsw_21_days              28.51     09-Dec-1982-17h00            343
TWAECsw_28_days              26.47     16-Dec-1982-16h00            350
TWAECsw_42_days              23.50     30-Dec-1982-13h00            364
TWAECsw_50_days              22.88     07-Jan-1983-15h00            372
TWAECsw_100_days             22.05     26-Feb-1983-12h00            422
* ------------------------------------------------------------------------------
```

4.2.8 Running SWAN

As explained previously SWAN is not part of FOUCS SWASH but must be called separately using the SWAN icon. The model opens with the screen presented in Figure 41. The model guides the user through risk mitigation via a stepwise procedure.

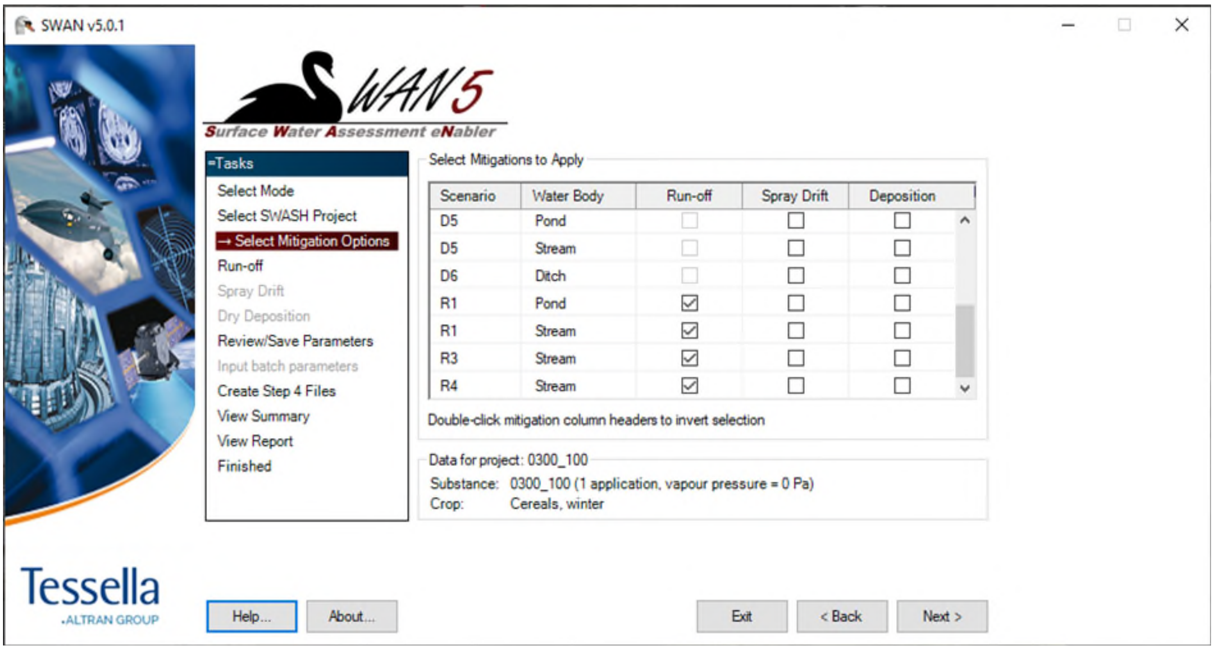
First an existing source SWASH project have to be selected where all runs have been performed. It is the same folder as defined previously when running SWASH (see Figure 24). Then a second folder has to be created or selected for the mitigation results. Both folders can be entered using the right buttons marked in the figure.

Figure 41: SWAN: Initial screen



After moving to the next step (button "next") a form with several mitigation options for the compound is presented. Only "Run-off" mitigation would be relevant for veterinary products since the compounds are incorporated and applied without assuming spray drift. Also deposition after volatilisation is not considered to occur. Consequently, only "Run-off" should be checked (see Figure 42).

Figure 42: SWAN: Mitigation options



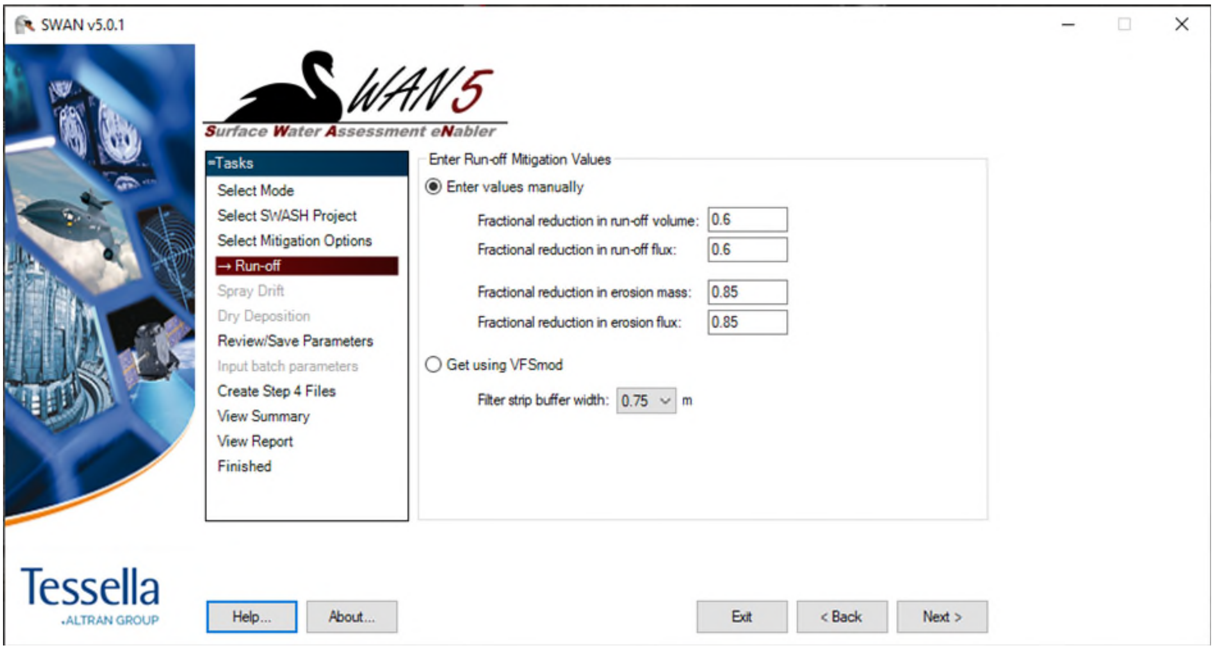
After leaving this form via the button "next", the run-off mitigation has to be specified (see Figure 43). As explained previously in chapter 2.3 there are two options either

- Constant reduction factors dependent on the width of the buffer strip (reduction independently on the run-off/erosion event). The factors are suggested by the FOCUS landscape and mitigation group (FOCUS 2007). Respective factors are available for 10 m and 20 m buffer widths.

- Reduction factors calculated with the mechanistic model VFSMOD. The factors are dependent on various parameter such as the width of the buffer strip, the run-off event and the soil conditions (e.g., moisture) on the buffer strip. VFSMOD is able to calculate reduction for every distance (not only 10 m and 20 m). However, so far, there are no recommendations that VFSMOD should be used for veterinary compounds.

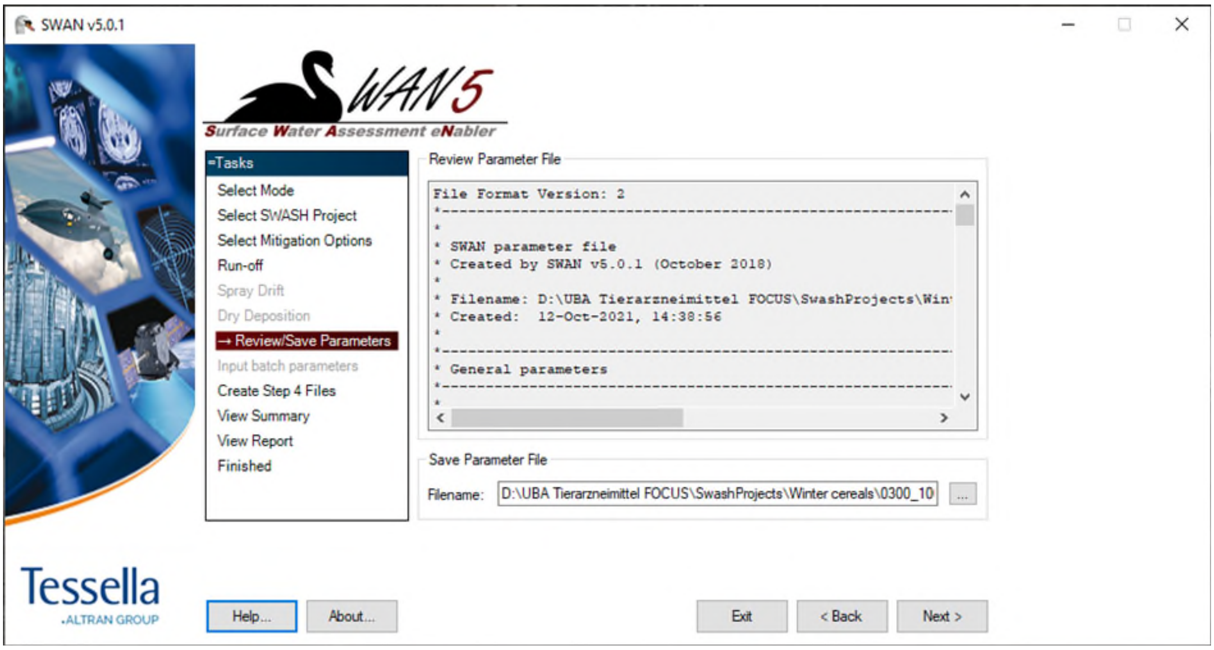
After the information in the form has been addressed use the button next to continue.

Figure 43: SWAN: Specifying run-off mitigation



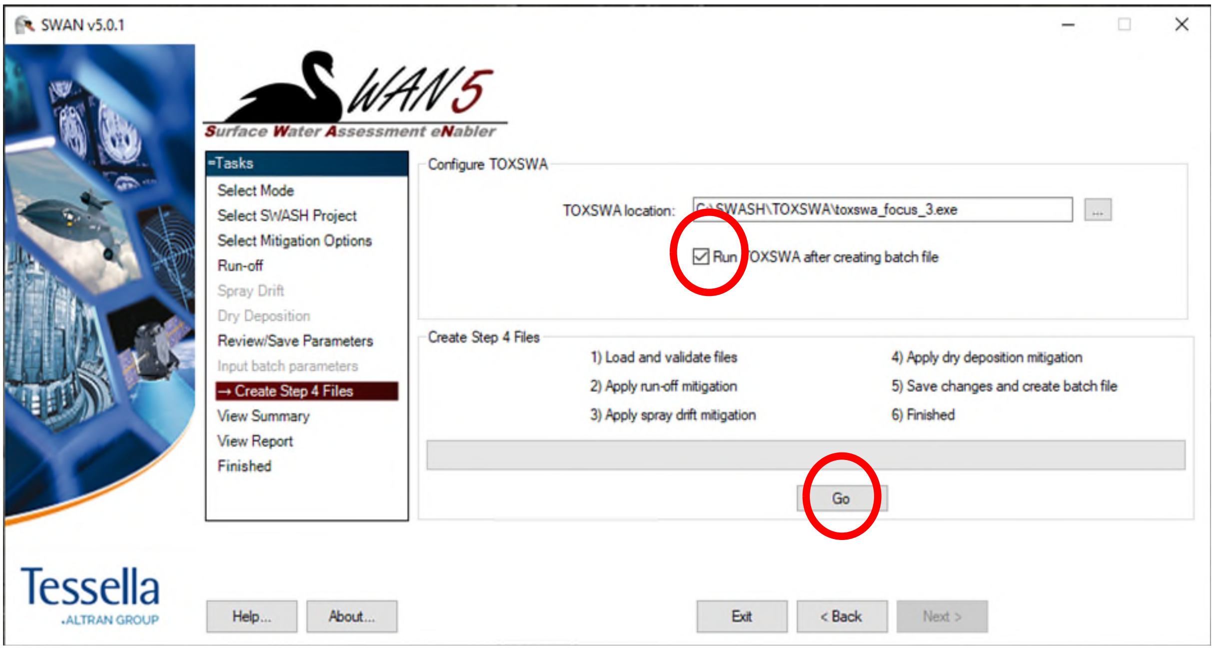
The form presented in Figure 44 will load. Here you could simply accept all setting and continue with “next”.

Figure 44: SWAN: Summarising the selected mitigation measures



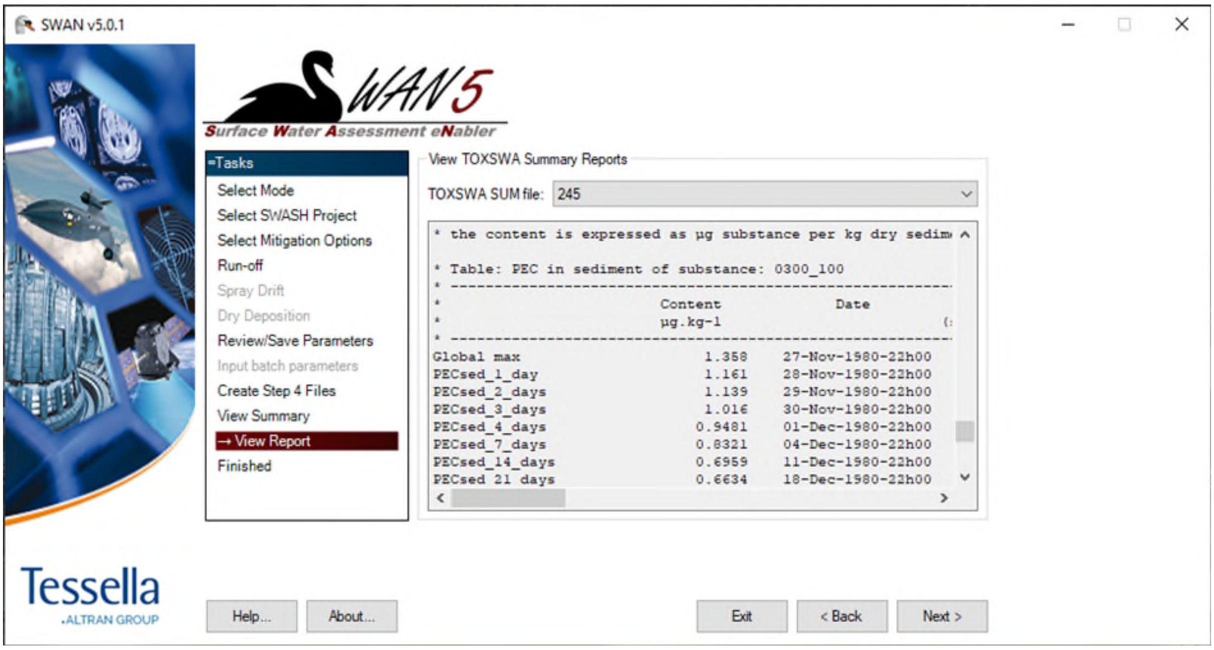
In the following step (see Figure 45) all input parameters for TOXSWA will be prepared. If the model VFSMOD has been selected previously, it may take some time before all TOXSWA input values are ready.

Figure 45: SWAN: Preparing the TOXSWA simulation



In the final step the results can be evaluated as shown in Figure 46. Using SWAN may be helpful in recalculating risk quotients considering risk mitigation measures. However, for successful implementation, all other criteria for risk mitigation measures according to the reflection paper (EMA 2011) also need to be considered.

Figure 46: SWAN: Viewing results of the mitigation measure



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A Appendix: Results of FOCUS GW simulations

A.1 Summary of all FOCUS PEARL simulations in winter cereals

Table 38: Results of FOCUS groundwater scenarios for compounds with low sorption (Kfoc = 1 L/kg) when 1 kg/ha were incorporated 14 days before crop emergence of winter cereals (FOCUS PEARL 5.5.5, concentrations in µg/L)

DegT50 (d)	1	3	10	30	100	300
Châteaudun	0.001	0.605	20.715	111.228	386.992	707.023
Hamburg	0.172	14.959	110.398	315.554	530.003	621.420
Jokioinen	0.023	8.069	137.800	404.063	628.431	776.467
Kremsmünster	0.022	2.600	38.602	125.328	228.638	279.503
Okehampton	0.013	2.428	44.681	142.962	236.260	282.853
Piacenza	0.068	3.473	33.862	106.544	274.596	442.690
Porto	0.011	3.294	41.848	106.858	183.269	245.734
Sevilla	0.000	0.000	0.323	7.834	148.593	539.702
Thiva	0.001	0.615	13.801	77.261	408.502	1067.269

Table 39: Results of FOCUS groundwater scenarios for compounds with low sorption (Kfoc = 3 L/kg) when 1 kg/ha were incorporated 14 days before crop emergence of winter cereals (FOCUS PEARL 5.5.5, concentrations in µg/L)

DegT50 (d)	1	3	10	30	100	300
Châteaudun	0.000	0.412	16.079	98.717	358.636	698.865
Hamburg	0.086	9.731	84.851	251.842	498.078	588.603
Jokioinen	0.011	5.030	98.441	330.469	602.628	768.845
Kremsmünster	0.013	2.146	35.090	113.980	226.603	282.746
Okehampton	0.007	1.780	38.853	132.320	223.879	269.462
Piacenza	0.046	2.523	29.516	97.200	251.394	423.104
Porto	0.005	2.518	36.567	100.353	175.611	238.845
Sevilla	0.000	0.000	0.163	6.356	132.310	519.097
Thiva	0.000	0.430	10.802	66.395	382.960	1022.958

Table 40: Results of FOCUS groundwater scenarios for compounds with low sorption (Kfoc = 10 L/kg) when 1 kg/ha were incorporated 14 days before crop emergence of winter cereals (FOCUS PEARL 5.5.5, concentrations in µg/L)

DegT50 (d)	1	3	10	30	100	300
Châteaudun	0.000	0.099	6.251	64.802	296.762	608.367
Hamburg	0.009	3.176	44.605	159.607	380.402	500.779
Jokioinen	0.000	1.241	36.590	201.499	507.084	753.501
Kremsmünster	0.002	0.952	17.168	79.791	201.448	280.527
Okehampton	0.001	0.719	26.354	102.174	197.813	240.481
Piacenza	0.011	0.921	17.523	77.807	186.311	377.154
Porto	0.000	1.228	25.549	76.720	158.731	233.453
Sevilla	0.000	0.000	0.000	3.060	85.823	485.246
Thiva	0.000	0.117	4.320	41.432	316.953	844.151

Table 41: Results of FOCUS groundwater scenarios for compounds with low sorption (Kfoc = 30 L/kg) when 1 kg/ha were incorporated 14 days before crop emergence of winter cereals (FOCUS PEARL 5.5.5, concentrations in µg/L)

DegT50 (d)	1	3	10	30	100	300
Châteaudun	0.000	0.000	0.391	21.832	160.537	470.156
Hamburg	0.000	0.106	7.397	58.054	224.611	399.816
Jokioinen	0.000	0.009	4.243	53.057	258.320	540.168
Kremsmünster	0.000	0.047	2.778	36.282	139.116	238.486
Okehampton	0.000	0.099	7.383	49.167	137.473	201.819
Piacenza	0.000	0.058	3.459	30.117	124.268	315.889
Porto	0.000	0.094	7.111	38.581	107.861	203.880
Sevilla	0.000	0.000	0.000	0.331	28.815	288.164
Thiva	0.000	0.002	0.148	11.863	184.696	658.536

Table 42: Results of FOCUS groundwater scenarios for compounds with low sorption (Kfoc = 100 L/kg) when 1 kg/ha were incorporated 14 days before crop emergence of winter cereals (FOCUS PEARL 5.5.5, concentrations in µg/L)

DegT50 (d)	1	3	10	30	100	300
Châteaudun	0.000	0.000	0.000	0.488	35.730	191.060
Hamburg	0.000	0.000	0.034	4.734	63.954	205.423
Jokioinen	0.000	0.000	0.002	1.747	44.677	192.625
Kremsmünster	0.000	0.000	0.015	2.816	46.933	154.410

DegT50 (d)	1	3	10	30	100	300
Okehampton	0.000	0.000	0.050	5.637	55.556	147.083
Piacenza	0.000	0.000	0.010	2.256	39.594	163.901
Porto	0.000	0.000	0.009	2.591	35.208	118.129
Sevilla	0.000	0.000	0.000	0.000	0.679	41.333
Thiva	0.000	0.000	0.000	0.117	31.253	300.893

Table 43: Results of FOCUS groundwater scenarios for compounds with moderate sorption (Kfoc = 300 L/kg) when 1 kg/ha were incorporated 14 days before crop emergence of winter cereals (FOCUS PEARL 5.5.5, concentrations in µg/L)

DegT50 (d)	1	3	10	30	100	300
Châteaudun	0.000	0.000	0.000	0.000	0.771	37.170
Hamburg	0.000	0.000	0.000	0.010	5.001	62.770
Jokioinen	0.000	0.000	0.000	0.000	1.591	35.630
Kremsmünster	0.000	0.000	0.000	0.007	4.186	46.376
Okehampton	0.000	0.000	0.000	0.025	6.797	55.376
Piacenza	0.000	0.000	0.000	0.003	2.538	41.000
Porto	0.000	0.000	0.000	0.000	1.804	32.905
Sevilla	0.000	0.000	0.000	0.000	0.000	1.104
Thiva	0.000	0.000	0.000	0.000	0.169	37.897

Table 44: Results of FOCUS groundwater scenarios for compounds with strong sorption (Kfoc = 1000 L/kg) when 1 kg/ha were incorporated 14 days before crop emergence of winter cereals (FOCUS PEARL 5.5.5, concentrations in µg/L)

DegT50 (d)	1	3	10	30	100	300
Châteaudun	0.000	0.000	0.000	0.000	0.000	0.034
Hamburg	0.000	0.000	0.000	0.000	0.003	2.199
Jokioinen	0.000	0.000	0.000	0.000	0.000	0.000
Kremsmünster	0.000	0.000	0.000	0.000	0.002	1.772
Okehampton	0.000	0.000	0.000	0.000	0.013	3.840
Piacenza	0.000	0.000	0.000	0.000	0.001	1.323
Porto	0.000	0.000	0.000	0.000	0.000	0.514
Sevilla	0.000	0.000	0.000	0.000	0.000	0.000
Thiva	0.000	0.000	0.000	0.000	0.000	0.000

Table 45: Results of FOCUS groundwater scenarios for compounds with strong sorption (Kfoc = 3000 L/kg) when 1 kg/ha were incorporated 14 days before crop emergence of winter cereals (FOCUS PEARL 5.5.5, concentrations in µg/L)

DegT50 (d)	1	3	10	30	100	300
Châteaudun	0.000	0.000	0.000	0.000	0.000	0.000
Hamburg	0.000	0.000	0.000	0.000	0.000	0.000
Jokioinen	0.000	0.000	0.000	0.000	0.000	0.000
Kremsmünster	0.000	0.000	0.000	0.000	0.000	0.000
Okehampton	0.000	0.000	0.000	0.000	0.000	0.000
Piacenza	0.000	0.000	0.000	0.000	0.000	0.000
Porto	0.000	0.000	0.000	0.000	0.000	0.000
Sevilla	0.000	0.000	0.000	0.000	0.000	0.000
Thiva	0.000	0.000	0.000	0.000	0.000	0.000

Table 46: Rank of FOCUS groundwater scenarios for compounds with low sorption (Kfoc = 1 L/kg) when 1 kg/ha were incorporated 14 days before crop emergence of winter cereals (FOCUS PEARL 5.5.5, concentrations in µg/L)

DegT50 (d)	1	3	10	30	100	300
Châteaudun	8	8	7	5	4	3
Hamburg	1	1	2	2	2	4
Jokioinen	3	2	1	1	1	2
Kremsmünster	4	5	5	4	7	8
Okehampton	5	6	3	3	6	7
Piacenza	2	3	6	7	5	6
Porto	6	4	4	6	8	9
Sevilla	9	9	9	9	9	5
Thiva	7	7	8	8	3	1

Table 47: Rank of FOCUS groundwater scenarios for compounds with low sorption (Kfoc = 3 L/kg) when 1 kg/ha were incorporated 14 days before crop emergence of winter cereals (FOCUS PEARL 5.5.5, concentrations in µg/L)

DegT50 (d)	1	3	10	30	100	300
Châteaudun	8	8	7	6	4	3
Hamburg	1	1	2	2	2	4
Jokioinen	4	2	1	1	1	2
Kremsmünster	3	5	5	4	6	7

DegT50 (d)	1	3	10	30	100	300
Okehampton	5	6	3	3	7	8
Piacenza	2	3	6	7	5	6
Porto	6	4	4	5	8	9
Sevilla	9	9	9	9	9	5
Thiva	7	7	8	8	3	1

Table 48: Rank of FOCUS groundwater scenarios for compounds with low sorption (Kfoc = 10 L/kg) when 1 kg/ha were incorporated 14 days before crop emergence of winter cereals (FOCUS PEARL 5.5.5, concentrations in µg/L)

DegT50 (d)	1	3	10	30	100	300
Châteaudun	8	8	7	7	4	3
Hamburg	2	1	1	2	2	4
Jokioinen	5	2	2	1	1	2
Kremsmünster	3	4	6	4	5	7
Okehampton	4	6	3	3	6	8
Piacenza	1	5	5	5	7	6
Porto	6	3	4	6	8	9
Sevilla	9	9	9	9	9	5
Thiva	7	7	8	8	3	1

Table 49: Rank of FOCUS groundwater scenarios for compounds with low sorption (Kfoc = 30 L/kg) when 1 kg/ha were incorporated 14 days before crop emergence of winter cereals (FOCUS PEARL 5.5.5, concentrations in µg/L)

DegT50 (d)	1	3	10	30	100	300
Châteaudun	5	8	7	7	4	3
Hamburg	1	1	1	1	2	4
Jokioinen	5	6	4	2	1	2
Kremsmünster	5	5	6	5	5	7
Okehampton	4	2	2	3	6	9
Piacenza	2	4	5	6	7	5
Porto	3	3	3	4	8	8
Sevilla	5	9	9	9	9	6
Thiva	5	7	8	8	3	1

Table 50: Rank of FOCUS groundwater scenarios for compounds with low sorption (Kfoc = 100 L/kg) when 1 kg/ha were incorporated 14 days before crop emergence of winter cereals (FOCUS PEARL 5.5.5, concentrations in µg/L)

DegT50 (d)	1	3	10	30	100	300
Châteaudun	1	1	7	7	6	4
Hamburg	1	1	2	2	1	2
Jokioinen	1	1	6	6	4	3
Kremsmünster	1	1	3	3	3	6
Okehampton	1	1	1	1	2	7
Piacenza	1	1	4	5	5	5
Porto	1	1	5	4	7	8
Sevilla	1	1	8	9	9	9
Thiva	1	1	8	8	8	1

Table 51: Rank of FOCUS groundwater scenarios for compounds with moderate sorption (Kfoc = 300 L/kg) when 1 kg/ha were incorporated 14 days before crop emergence of winter cereals (FOCUS PEARL 5.5.5, concentrations in µg/L)

DegT50 (d)	1	3	10	30	100	300
Châteaudun	1	1	1	7	7	6
Hamburg	1	1	1	2	2	1
Jokioinen	1	1	1	6	6	7
Kremsmünster	1	1	1	3	3	3
Okehampton	1	1	1	1	1	2
Piacenza	1	1	1	4	4	4
Porto	1	1	1	5	5	8
Sevilla	1	1	1	8	9	9
Thiva	1	1	1	8	8	5

Table 52: Rank of FOCUS groundwater scenarios for compounds with strong sorption (Kfoc = 1000 L/kg) when 1 kg/ha were incorporated 14 days before crop emergence of winter cereals (FOCUS PEARL 5.5.5, concentrations in µg/L)

DegT50 (d)	1	3	10	30	100	300
Châteaudun	1	1	1	1	6	6
Hamburg	1	1	1	1	2	2
Jokioinen	1	1	1	1	6	7

DegT50 (d)	1	3	10	30	100	300
Kremsmünster	1	1	1	1	3	3
Okehampton	1	1	1	1	1	1
Piacenza	1	1	1	1	4	4
Porto	1	1	1	1	5	5
Sevilla	1	1	1	1	6	9
Thiva	1	1	1	1	6	8

Table 53: Rank of FOCUS groundwater scenarios for compounds with strong sorption (Kfoc = 3000 L/kg) when 1 kg/ha were incorporated 14 days before crop emergence of winter cereals (FOCUS PEARL 5.5.5, concentrations in µg/L)

DegT50 (d)	1	3	10	30	100	300
Châteaudun	1	1	1	1	1	3
Hamburg	1	1	1	1	1	3
Jokioinen	1	1	1	1	1	3
Kremsmünster	1	1	1	1	1	3
Okehampton	1	1	1	1	1	2
Piacenza	1	1	1	1	1	1
Porto	1	1	1	1	1	3
Sevilla	1	1	1	1	1	3
Thiva	1	1	1	1	1	3

A.2 Summary of all FOCUS PEARL simulations in maize

Table 54: Results of FOCUS groundwater scenarios for compounds with low sorption (Kfoc = 1 L/kg) when 1 kg/ha were incorporated 14 days before crop emergence of maize (FOCUS PEARL 5.5.5, concentrations in µg/L)

DegT50 (d)	1	3	10	30	100	300
Châteaudun	0.000	0.000	1.550	53.686	236.160	377.637
Hamburg	0.000	0.008	7.115	108.469	344.694	490.832
Jokioinen						
Kremsmünster	0.000	0.034	5.511	65.419	193.984	277.346
Okehampton	0.000	0.038	6.123	61.775	173.108	250.909
Piacenza	0.000	0.005	1.648	33.582	210.140	390.657
Porto	0.000	0.002	0.723	20.850	105.714	161.508
Sevilla	0.000	0.000	0.011	4.593	117.058	436.181
Thiva	0.000	0.000	0.112	24.941	298.387	682.978

Table 55: Results of FOCUS groundwater scenarios for compounds with low sorption (Kfoc = 3 L/kg) when 1 kg/ha were incorporated 14 days before crop emergence of maize (FOCUS PEARL 5.5.5, concentrations in µg/L)

DegT50 (d)	1	3	10	30	100	300
Châteaudun	0.000	0.000	1.216	48.506	228.458	374.546
Hamburg	0.000	0.004	5.692	98.595	336.489	491.618
Jokioinen						
Kremsmünster	0.000	0.020	4.396	59.228	186.824	271.678
Okehampton	0.000	0.023	5.068	56.383	168.603	244.726
Piacenza	0.000	0.003	1.326	28.840	193.525	373.435
Porto	0.000	0.001	0.487	17.828	96.827	156.158
Sevilla	0.000	0.000	0.008	4.104	109.362	416.170
Thiva	0.000	0.000	0.088	22.405	285.420	670.971

Table 56: Results of FOCUS groundwater scenarios for compounds with low sorption (Kfoc = 10 L/kg) when 1 kg/ha were incorporated 14 days before crop emergence of maize (FOCUS PEARL 5.5.5, concentrations in µg/L)

DegT50 (d)	1	3	10	30	100	300
Châteaudun	0.000	0.000	0.554	32.289	200.161	362.214
Hamburg	0.000	0.001	2.670	69.452	293.534	470.525

DegT50 (d)	1	3	10	30	100	300
Jokioinen						
Kremsmünster	0.000	0.003	2.100	42.603	170.007	258.143
Okehampton	0.000	0.005	2.799	43.118	150.433	227.909
Piacenza	0.000	0.000	0.637	19.604	159.897	339.902
Porto	0.000	0.000	0.183	10.934	79.549	152.707
Sevilla	0.000	0.000	0.004	2.677	89.589	388.820
Thiva	0.000	0.000	0.037	15.244	242.782	628.910

Table 57: Results of FOCUS groundwater scenarios for compounds with low sorption (Kfoc = 30 L/kg) when 1 kg/ha were incorporated 14 days before crop emergence of maize (FOCUS PEARL 5.5.5, concentrations in µg/L)

DegT50 (d)	1	3	10	30	100	300
Châteaudun	0.000	0.000	0.059	11.791	126.095	283.026
Hamburg	0.000	0.000	0.331	22.839	175.492	368.409
Jokioinen						
Kremsmünster	0.000	0.000	0.428	17.840	120.721	232.705
Okehampton	0.000	0.000	0.662	21.020	106.730	192.309
Piacenza	0.000	0.000	0.094	9.158	108.102	306.059
Porto	0.000	0.000	0.014	4.149	52.958	132.611
Sevilla	0.000	0.000	0.000	0.779	48.556	286.460
Thiva	0.000	0.000	0.003	5.021	141.337	546.774

Table 58: Results of FOCUS groundwater scenarios for compounds with low sorption (Kfoc = 100 L/kg) when 1 kg/ha were incorporated 14 days before crop emergence of maize (FOCUS PEARL 5.5.5, concentrations in µg/L)

DegT50 (d)	1	3	10	30	100	300
Châteaudun	0.000	0.000	0.000	0.434	33.489	161.730
Hamburg	0.000	0.000	0.001	1.403	47.488	191.324
Jokioinen						
Kremsmünster	0.000	0.000	0.001	1.211	36.369	142.820
Okehampton	0.000	0.000	0.004	2.241	43.380	128.467
Piacenza	0.000	0.000	0.001	0.959	32.090	167.417
Porto	0.000	0.000	0.000	0.206	17.116	77.273
Sevilla	0.000	0.000	0.000	0.003	5.720	103.761

DegT50 (d)	1	3	10	30	100	300
Thiva	0.000	0.000	0.000	0.056	27.000	244.360

Table 59: Results of FOCUS groundwater scenarios for compounds with moderate sorption (Kfoc = 300 L/kg) when 1 kg/ha were incorporated 14 days before crop emergence of maize (FOCUS PEARL 5.5.5, concentrations in µg/L)

DegT50 (d)	1	3	10	30	100	300
Châteaudun	0.000	0.000	0.000	0.000	1.378	42.795
Hamburg	0.000	0.000	0.000	0.002	3.513	57.311
Jokioinen						
Kremsmünster	0.000	0.000	0.000	0.002	3.111	42.329
Okehampton	0.000	0.000	0.000	0.006	4.853	50.322
Piacenza	0.000	0.000	0.000	0.001	2.832	43.414
Porto	0.000	0.000	0.000	0.000	0.803	24.037
Sevilla	0.000	0.000	0.000	0.000	0.006	4.318
Thiva	0.000	0.000	0.000	0.000	0.367	42.496

Table 60: Results of FOCUS groundwater scenarios for compounds with strong sorption (Kfoc = 1000 L/kg) when 1 kg/ha were incorporated 14 days before crop emergence of maize (FOCUS PEARL 5.5.5, concentrations in µg/L)

DegT50 (d)	1	3	10	30	100	300
Châteaudun	0.000	0.000	0.000	0.000	0.000	0.425
Hamburg	0.000	0.000	0.000	0.000	0.002	1.844
Jokioinen						
Kremsmünster	0.000	0.000	0.000	0.000	0.001	1.529
Okehampton	0.000	0.000	0.000	0.000	0.008	3.487
Piacenza	0.000	0.000	0.000	0.000	0.001	1.832
Porto	0.000	0.000	0.000	0.000	0.000	0.399
Sevilla	0.000	0.000	0.000	0.000	0.000	0.000
Thiva	0.000	0.000	0.000	0.000	0.000	0.067

Table 61: Results of FOCUS groundwater scenarios for compounds with strong sorption (Kfoc = 3000 L/kg) when 1 kg/ha were incorporated 14 days before crop emergence of maize (FOCUS PEARL 5.5.5, concentrations in µg/L)

DegT50 (d)	1	3	10	30	100	300
Châteaudun	0.000	0.000	0.000	0.000	0.000	0.000
Hamburg	0.000	0.000	0.000	0.000	0.000	0.000
Jokioinen						
Kremsmünster	0.000	0.000	0.000	0.000	0.000	0.000
Okehampton	0.000	0.000	0.000	0.000	0.000	0.000
Piacenza	0.000	0.000	0.000	0.000	0.000	0.000
Porto	0.000	0.000	0.000	0.000	0.000	0.000
Sevilla	0.000	0.000	0.000	0.000	0.000	0.000
Thiva	0.000	0.000	0.000	0.000	0.000	0.000

Table 62: Relative difference (%) of concentrations for applications to maize instead of winter cereals for compounds with low sorption (Kfoc=1 L/kg).

Results of FOCUS groundwater scenarios when 1 kg/ha were incorporated 14 days before crop emergence (FOCUS PEARL 5.5.5)

DegT50 (d)	1	3	10	30	100	300
Châteaudun	n.a.	-99.9	-92.5	-51.7	-39.0	-46.6
Hamburg	-100.0	-99.9	-93.6	-65.6	-35.0	-21.0
Jokioinen	-100.0	-100.0	-100.0	-100.0	-100.0	-100.0
Kremsmünster	-99.8	-98.7	-85.7	-47.8	-15.2	-0.8
Okehampton	-98.6	-98.4	-86.3	-56.8	-26.7	-11.3
Piacenza	-100.0	-99.9	-95.1	-68.5	-23.5	-11.8
Porto	-100.0	-100.0	-98.3	-80.5	-42.3	-34.3
Sevilla	n.a.	n.a.	-96.7	-41.4	-21.2	-19.2
Thiva	n.a.	-100.0	-99.2	-67.7	-27.0	-36.0

Table 63: Relative difference (%) of concentrations for applications to maize instead of winter cereals for compounds with low sorption (Kfoc = 3 L/kg).

Results of FOCUS groundwater scenarios when 1 kg/ha were incorporated 14 days before crop emergence (FOCUS PEARL 5.5.5)

DegT50 (d)	1	3	10	30	100	300
Châteaudun	n.a.	-100.0	-92.4	-50.9	-36.3	-46.4
Hamburg	-100.0	-100.0	-93.3	-60.9	-32.4	-16.5

DegT50 (d)	1	3	10	30	100	300
Jokioinen	-100.0	-100.0	-100.0	-100.0	-100.0	-100.0
Kremsmünster	-99.9	-99.1	-87.5	-48.0	-17.6	-3.9
Okehampton	-99.1	-98.7	-87.0	-57.4	-24.7	-9.2
Piacenza	-100.0	-99.9	-95.5	-70.3	-23.0	-11.7
Porto	-100.0	-100.0	-98.7	-82.2	-44.9	-34.6
Sevilla	n.a.	n.a.	-94.8	-35.4	-17.3	-19.8
Thiva	n.a.	-100.0	-99.2	-66.3	-25.5	-34.4

Table 64: Relative difference (%) of concentrations for applications to maize instead of winter cereals for compounds with low sorption (Kfoc = 10 L/kg).

Results of FOCUS groundwater scenarios when 1 kg/ha were incorporated 14 days before crop emergence (FOCUS PEARL 5.5.5)

DegT50 (d)	1	3	10	30	100	300
Châteaudun	n.a.	-100.0	-91.1	-50.2	-32.6	-40.5
Hamburg	-100.0	-100.0	-94.0	-56.5	-22.8	-6.0
Jokioinen						
Kremsmünster	-100.0	-99.7	-87.8	-46.6	-15.6	-8.0
Okehampton	n.a.	-99.3	-89.4	-57.8	-24.0	-5.2
Piacenza	-100.0	-100.0	-96.4	-74.8	-14.2	-9.9
Porto	n.a.	-100.0	-99.3	-85.7	-49.9	-34.6
Sevilla	n.a.	n.a.	n.a.	-12.5	4.4	-19.9
Thiva	n.a.	-100.0	-99.1	-63.2	-23.4	-25.5

Table 65: Relative difference (%) of concentrations for applications to made to maize instead of winter cereals for compounds with low sorption (Kfoc = 30 L/kg).

Results of FOCUS groundwater scenarios when 1 kg/ha were incorporated 14 days before crop emergence (FOCUS PEARL 5.5.5)

DegT50 (d)	1	3	10	30	100	300
Châteaudun	n.a.	n.a.	-84.8	-46.0	-21.5	-39.8
Hamburg	n.a.	-100.0	-95.5	-60.7	-21.9	-7.9
Jokioinen						
Kremsmünster	n.a.	-100.0	-84.6	-50.8	-13.2	-2.4
Okehampton	n.a.	-99.9	-91.0	-57.2	-22.4	-4.7
Piacenza	n.a.	-100.0	-97.3	-69.6	-13.0	-3.1

DegT50 (d)	1	3	10	30	100	300
Porto	n.a.	-100.0	-99.8	-89.2	-50.9	-35.0
Sevilla	n.a.	n.a.	n.a.	135.5	68.5	-0.6
Thiva	n.a.	-100.0	-97.8	-57.7	-23.5	-17.0

Table 66: Relative difference (%) of concentrations for applications made to maize instead of winter cereals for compounds with low sorption (Kfoc = 100 L/kg).

Results of FOCUS groundwater scenarios when 1 kg/ha were incorporated 14 days before crop emergence (FOCUS PEARL 5.5.5)

DegT50 (d)	1	3	10	30	100	300
Châteaudun	n.a.	n.a.	n.a.	-11.2	-6.3	-15.4
Hamburg	n.a.	n.a.	-98.2	-70.4	-25.7	-6.9
Jokioinen						
Kremsmünster	n.a.	n.a.	-95.5	-57.0	-22.5	-7.5
Okehampton	n.a.	n.a.	-92.6	-60.3	-21.9	-12.7
Piacenza	n.a.	n.a.	-93.5	-57.5	-19.0	2.1
Porto	n.a.	n.a.	-100.0	-92.0	-51.4	-34.6
Sevilla	n.a.	n.a.	n.a.	n.a.	742.9	151.0
Thiva	n.a.	n.a.	n.a.	-52.3	-13.6	-18.8

Table 67: Relative difference (%) of concentrations for applications to maize instead of winter cereals for compounds with moderate sorption (Kfoc = 300 L/kg).

Results of FOCUS groundwater scenarios when 1 kg/ha were incorporated 14 days before crop emergence (FOCUS PEARL 5.5.5)

DegT50 (d)	1	3	10	30	100	300
Châteaudun	n.a.	n.a.	n.a.	n.a.	78.6	15.1
Hamburg	n.a.	n.a.	n.a.	-76.5	-29.8	-8.7
Jokioinen						
Kremsmünster	n.a.	n.a.	n.a.	-71.6	-25.7	-8.7
Okehampton	n.a.	n.a.	n.a.	-74.6	-28.6	-9.1
Piacenza	n.a.	n.a.	n.a.	-63.9	11.6	5.9
Porto	n.a.	n.a.	n.a.	n.a.	-55.5	-27.0
Sevilla	n.a.	n.a.	n.a.	n.a.	n.a.	291.2
Thiva	n.a.	n.a.	n.a.	n.a.	117.1	12.1

Table 68: Relative difference (%) of concentrations for applications to maize instead of winter cereals for compounds with strong sorption (Kfoc = 1000 L/kg).

Results of FOCUS groundwater scenarios when 1 kg/ha were incorporated 14 days before crop emergence (FOCUS PEARL 5.5.5)

DegT50 (d)	1	3	10	30	100	300
Châteaudun	n.a.	n.a.	n.a.	n.a.	n.a.	1168.2
Hamburg	n.a.	n.a.	n.a.	n.a.	-35.5	-16.2
Jokioinen						
Kremsmünster	n.a.	n.a.	n.a.	n.a.	-36.8	-13.7
Okehampton	n.a.	n.a.	n.a.	n.a.	-33.4	-9.2
Piacenza	n.a.	n.a.	n.a.	n.a.	n.a.	38.5
Porto	n.a.	n.a.	n.a.	n.a.	n.a.	-22.3
Sevilla	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
Thiva	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.

Table 69: Relative difference (%) of concentrations for applications to maize instead of winter cereals for compounds with strong sorption (Kfoc = 3000 L/kg).

Results of FOCUS groundwater scenarios when 1 kg/ha were incorporated 14 days before crop emergence (FOCUS PEARL 5.5.5)

DegT50 (d)	1	3	10	30	100	300
Châteaudun	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
Hamburg	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
Jokioinen						
Kremsmünster	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
Okehampton	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
Piacenza	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
Porto	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
Sevilla	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
Thiva	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.