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# Recommendations for Simulations to Predict Environmental Concentrations of Active Substances of Plant Protection Products and their Metabolites in Groundwater (PECgw) in the National Assessment for Authorisation in Germany

## Part 1: Tier 1 and Tier 2

# Empfehlungen für Simulationen zur Prognose der Konzentration von Pflanzenschutzmittelwirkstoffen und -metaboliten im Grundwasser (PECgw) in der nationalen Bewertung für die Zulassung in Deutschland

## Teil 1: Stufe 1 und Stufe 2

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# 1 Abstract

In the national assessment for authorisation in Germany the leaching behaviour of a plant protection product is determined in a stepwise procedure in accordance with FOCUS groundwater report (2009). The recommendations given in this paper here are related to tier 1 and tier 2, only. A further publication is planned for the tier 3 and tier 4 assessments in accordance with the principles provided by FOCUS.

The tier 1 leaching assessment in the EU evaluation process is based on the nine FOCUS (2009) standard groundwater scenarios. In the member state evaluation for Germany, a subset of the standard scenarios with climatic and soil conditions found to be relevant for Germany are taken into account (Hamburg and Kremsmünster). The soils of the two scenarios cover the pH-range of agricultural soils and allow the pH-dependent behaviour of compounds to be addressed.

For the parameterisation of the degradation behaviour of an active substance and its metabolites in soil the recommendations of FOCUS should be followed. Normalised degradation rates may be taken from either laboratory or from field dissipation studies.

For the parameterisation of the sorption behaviour of an active substance and its metabolites in soil the recommendations of FOCUS should be considered.

With respect to the correlation of degradation and/or sorption behaviour to soil properties (pH, OC) further detailed recommendations are provided to facilitate the selection of conservative sorption parameters for leaching assessment. Proposals and detailed schemes for the handling of the DT50 and Kfoc values (including their variability) are given.

Further recommendations are given in this paper on how to use other modelling parameters e.g. crop rotation, plant uptake factor, formation of metabolites, correlations / multicorrelations of substance parameters to soil properties, and application of statistical methods.

Tier 2 of the leaching assessment consists of more refined modelling approaches. This includes providing data on specific processes e.g. surface degradation or non-equilibrium sorption or alternatively the use of refined scenarios. Refined scenarios are appropriate when the standard tier 1 scenarios are not representative of a specific crop or the relationship between compound and scenario properties has to be considered specifically.

Although all models tested under FOCUS may be suitable in principle, it is recommended to use the most recent officially released version of the FOCUS PELMO model for submissions in Germany.

**Key words**: risk assessment, groundwater, plant protection products, predicted environmental concentration, simulation model, FOCUS PELMO, national authorisation, leaching behaviour, active substance, metabolite

**Abbreviations**: BBCH; BBA, Biologische Bundesanstalt;, Bundessortenamt und CHemische Industrie; CEC, cation exchange capacity; Corg, organic carbon content; DegT50, degradation half life time; DT50, half life time; CV, coefficient of variation; ff, formation fraction; FOCUS, FOrum for the Co-ordination of pesticide fate models and their USe; GAP, Good Agricultural Practice; Kf, Freundlich adsorption coefficient; logKow, octanol / water partition coefficient; OC, organic carbon content of a soil; PEC, predicted environmental concentration; PECgw, Predicted Environmental Concentration in Groundwater; PUF, plant uptake factor; QSAR, quantitative structure-activity relationship; TSCF, transpiration stream concentration factor

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## 2 Zusammenfassung

Im Rahmen des nationalen Zulassungsverfahrens für Pflanzenschutzmittel in Deutschland wird das Versickerungsverhalten von Wirkstoffen und Metaboliten in einem schrittweisen Verfahren nach FOCUS geprüft.

Die Stufe 1 in der EU-Wirkstoffprüfung basiert auf den neun in den FOCUS Groundwater Reports beschriebenen Standardszenarien. Die FOCUS-Szenarien „Hamburg" und „Kremsmünster" werden im Hinblick auf die klimatischen und pedologischen Bedingungen als relevant für das Deutsche Zulassungsverfahren betrachtet. Die Böden dieser beiden Szenarien decken weitgehend die pH-Bereiche landwirtschaftlicher Böden ab und erlauben es daher, die pH-Abhängigkeit des Umweltverhaltens von Pflanzenschutzmitteln in der nationalen Bewertung einzubeziehen.

Die Parametrisierung des Abbau- und Transformationsverhaltens sowie der Sorption von Wirksubstanzen und Metaboliten erfolgt nach FOCUS. Normalisierte Abbauraten können dabei entweder aus Labor- oder Freilandstudien stammen.

Im Hinblick auf die Korrelation des Abbau- und/oder Sorptionsverhaltens zu Bodeneigenschaften, wie pH oder OC, werden detaillierte Vorgaben gemacht, um die Auswahl von konservativen Parametern für eine Abschätzung des Versickerungsverhaltens zu ermöglichen, wobei auch die Parametervariabilität zu beachten ist.

Es werden Empfehlungen gegeben, wie entsprechende Modellierungsparameter wie Adsorption, Fruchtwechsel, Aufnahme durch die Pflanze, Abbauprodukte und deren Entstehung, Prüfung auf Existenz von Korrelationen zwischen einzelnen Parametern sowie die statistischen Methoden zur Prüfung auf Signifikanz anzuwenden sind.

Des Weiteren wird empfohlen, die neueste veröffentliche Version von FOCUS PELMO für entsprechende Submissions in Deutschland anzuwenden.

Stufe 2 beinhaltet verfeinerte Modellparameter. Einerseits werden hierbei spezifische Prozesse, wie Abbau auf Oberflächen oder die kinetische Sorption betrachtet und andererseits spezifische Szenarien in Betracht gezogen, wenn die Standardszenarien nicht repräsentativ sind.

In dieser Publikation werden nur die Stufen 1 und 2 im Rahmen der nationalen Bewertung für die Pflanzenschutzmittelzulassung betrachtet. Es ist geplant, in einer weiteren Veröffentlichung auch die anderen Verfahrensschritte (Stufe 3 und 4) unter Berücksichtigung der in FOCUS beschriebenen Grundsätze auszugestalten.

**Stichwörter**: Risikobewertung, Grundwasser, Pflanzenschutzmittel, erwartete Umweltkonzentration, Simulationsmodell, FOCUS PELMO, nationale Zulassung, Versickerungsneigung, Wirkstoff, Metabolit

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## 3 Introduction

A new FOCUS report 'Assessing Potential for Movement of Active Substances and their Metabolites to Groundwater in the EU' (2009) was published, commented on by the EU member states, taken note of by the SCFCAH and is in place for EU submissions after launch by the EFSA version control group on the FOCUS website since April 2011

(http://viso.ei.jrc.it/focus/gw/index.html). This FOCUS (2009) report concerns the groundwater risk assessment of plant protection products and their degradation products in the EU as well as in the national assessment for authorisation procedure. The report is based upon the requirements and criteria of the Directive 91/414/EWG and subsequent regulation EC (No) 1107/2009. Advanced simulation models were introduced and evaluated to calculate predicted environmental concentrations (PEC) of active substances and their metabolites in groundwater. In addition, a tiered approach was developed to consider extended modelling options in the groundwater risk assessment (Figure 1).

A joint ecochemistry expert group formed by the Federal Environment Agency (UBA) and the German Agrochemical Industry Association (IVA) developed recommendations for the risk assessment in Germany that are based, as far as possible, on a harmonised assessment in the EU as described in FOCUS (2009).

The joint UBA / IVA group concludes that the latest version of the program FOCUS PELMO shall replace the previously used model PELMO 3.0 (described by Michalski et al. 2004a) for PECgw simulations in the national assessment for authorisation in Germany. An overview on the validation status of the PELMO model is given in Hardy et al. (2008). The scenario and parameter selection for tier 1 and tier 2 calculations adapted from FOCUS (2009) is presented in detail. Furthermore a proposal for the use of statistical methods is given.
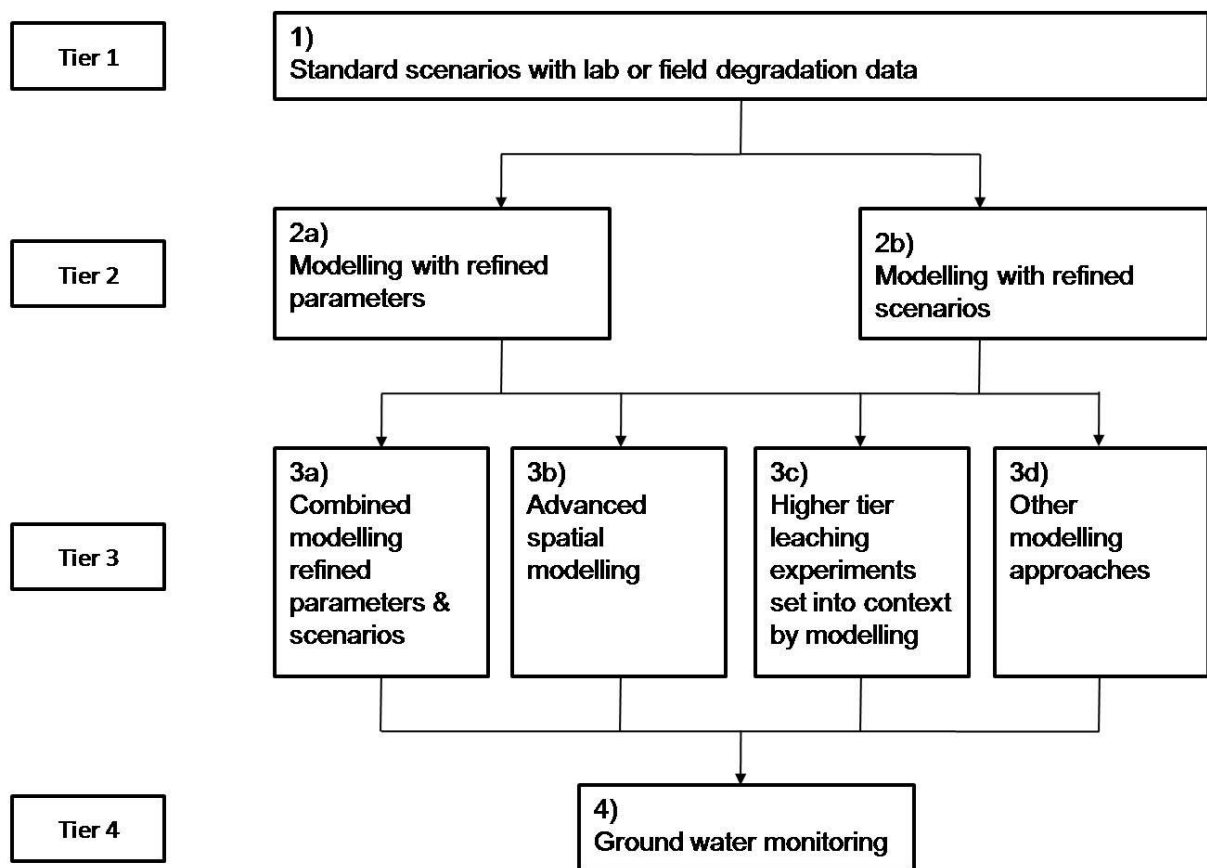


**Figure 1: Proposed generic tiered assessment scheme for groundwater (FOCUS, 2009)**

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## 4 Definition of the protection goal

As outlined in FOCUS (2009), the predicted environmental concentration in groundwater (PECgw) for active substances and relevant metabolites, identified according to guidances provided by EC DG Sanco/221/2000 -rev.10- final (2003) and Michalski et al. (2004b), should be below 0.1 µg/L.

The official FOCUS models and the European scenarios were set up to describe realistic worst case conditions with an overall vulnerability of the 90th percentile, approximated by using a 80th percentile value for soil and a 80th percentile value for weather (FOCUS Groundwater Scenarios in the EU Review of Active Substances, 2000). The use of the 90th percentile vulnerability, taking into account both spatial variability for soil and climatic conditions, and temporal variability on a multi-year basis, is seen as being consistent with definitions used in FOCUS (2000) and was agreed by the FOCUS Steering Committee and later by the Working ground water work group of FOCUS.

Accordingly, at tier 1 and 2 of the assessment scheme the regulatory relevant PECgw values are provided by the FOCUS models (80th percentile highest concentration in the averaging period representing a 90th percentile overall) at the FOCUS soil reference depth (1 m) in one of the scenarios relevant for Germany and is considered to be the regulatory relevant endpoint for both limit and guidance values, respectively.

## 5 Selection of scenarios for leaching assessment as a representative subset for Germany

The assessment of potential leaching to groundwater of active substances from plant protection products and / or their relevant metabolites in the EU is based on nine FOCUS standard scenarios which have been first described in FOCUS (2000) and are advanced in FOCUS (2009). The two scenarios Hamburg and Kremsmünster are the subset of the FOCUS standard scenarios with climatic and soil conditions found to be most relevant for a conservative groundwater risk assessment in the German national authorisation procedure. In particular, the soil pH-values of those scenarios cover acidic and basic conditions within a range relevant for agricultural soils. Thus the leaching behavior of compounds which show pH-dependent degradation and/or sorption can be determined in an appropriate and more realistic way by using both scenarios. If no evidence can be provided for pH-dependency it is recommended to use the reference scenario FOCUS Hamburg, only. The parameterisation of the scenarios is described in the chapters below.

## 6 Selection of simulation model for leaching assessment

According to FOCUS (2009) the groundwater assessment could be performed with different models (PEARL, PELMO, and PRZM). Although all models tested under FOCUS may be suitable in principle, it is recommended to use the most recent version of the FOCUS PELMO model which is released by the EFSA version control group (currently FOCUS PELMO 4.4.3) to calculate the PECgw of active substances and their relevant metabolites for national assessment for authorisation behaviour in Germany[1].

In general the principles for parameter selection are applied as outlined in FOCUS (2000, 2006, and 2009). The simulation models are under the model version control of EFSA (for-

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[1] In order to simplify intra-zonal mutual recognition within the central zone or inter-zonal mutual recognition it may be possible in special cases to submit calculations also with the PEARL model if the recommendations regarding parameterisation are followed.

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merly FOCUS) and can be downloaded from the FOCUS homepage
http://focus.jrc.ec.europa.eu

## 7   Statistical evaluation of dependency of pesticide behaviour from soil properties

A detailed procedure according to FOCUS (2009) was developed to determine dependency of pesticide degradation and/or sorption behaviour on different soil properties. In addition, patterns in the data may be characterised to account for variability and uncertainty in the observations.

Different parametric and non-parametric statistical tests are available to investigate the correlation between pesticide behaviour and soil properties. A rank correlation test evaluates the similarity of the ordering of data when ranked for each of the measured variables. It represents a reliable statistical test method when only a few values (e.g. 3 to 6) are available. So, since more than 3 sorption or degradation values are usually submitted (generally 5 to 10 values), the Kendall rank correlation test is proposed to be used to investigate the dependency of pesticide degradation and/or sorption behaviour on soil properties.

If the information regarding the direction of the correlation exists (e.g. a pesticide parameter is assumed to be positively correlated with a soil property, and a negative correlation can be excluded), the one sided Kendall test can be performed. Otherwise a two-sided Kendall test should be applied. Two values result from the statistical test: the Kendall-tau value (stringency of a correlation between 0 and 1) and the p-value (level of significance). A default significance level of 5 % is recommended to test for one sided correlations.

Harmonised and reproducible test results are necessary and it is found useful to provide notifiers and regulatory authorities with an agreed statistical tool. 'Excel' as part of the 'Microsoft® office' package is an often used program. However, because the Kendall rank correlation test is not a standard test in 'Excel' an additional tool is necessary. The Kendall rank correlation test is implemented in an 'Excel' sheet with the help of the package 'RExcel'. The R-tool (current version: RAndFriendsSetup2111V3.1-5-1) is freeware and can be downloaded from: http://rcom.univie.ac.at/.

The 'RExcel' tool, the manual for the installation and its use can be downloaded from the website of the Federal Office of Consumer Protection and Food Safety (link see BVL Homepage: http://www.bvl.bund.de/DE/Home/homepage_node.html; 2011).

The Kendall rank correlation test is implemented in an 'Excel'-based tool, 'Input-Decision 3' developed by Umweltbundesamt. It can also be downloaded from the BVL-website (see above). The version control for this tool is maintained via the BVL-website. Significant correlations between several substance and soil parameters, e.g. Kf and OC Kf and pH or DT50 and pH, etc. are testable simultaneously and endpoints for modelling can be derived, respectively. It is currently used by the German authorities and notifiers are encouraged to use the same tool.

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# 8 Recommendations for parameter selection in model calculation regarding leaching behaviour

## 8.1 Aerobic soil degradation

### 8.1.1 General requirements for the suitability and selection of the DT50 from laboratory studies and field studies

Laboratory DT50 values are used for tier 1 PECgw calculations at the beginning of the assessment.

DT50 values derived from field studies can subsequently be utilized as model input in the context of tier 1 simulation in cases where the PECgw using respective DT50 values from laboratory studies exceeds 0.1 µg/L.

According to Directive 91/414/EEC (including the annex II and III of the directive) at least 4 reliable DT50 values are required for the active substance and 3 values for metabolites from different soils. If sufficient data are available the selection of the DT50 values for modelling should follow the stepwise procedure as described in chapter 8.2.2. If less than 4 DT50 values from different soils are available for the active substance and less than 3 for the metabolites, the maximum DT50 value should be used.

In general, the kinetic evaluation of degradation values from laboratory and field studies and the selection of modelling endpoints should follow the actual recommendations of FOCUS kinetics (2006).

For use as input into simulation models to predict transport to groundwater depending on weather conditions the DT50 values need to be modelling endpoints (DegT50) according to FOCUS (2006) and thus need to be normalised to reference conditions (20 °C, pF2).

### 8.1.2 Criteria to accept laboratory studies

Degradation values derived from laboratory studies according to OECD 307 (OECD 2002) are acceptable in general. Results from older studies can be also accepted, if they follow the Guidelines BBA IV 4-1 (1986), USEPA 162-1 (1985), SETAC (1995).

Laboratory studies with experimental artefacts are invalid and should be excluded from further consideration in simulation calculations. A justification for exclusion has to be provided.

DT50 values from studies that are experimentally valid but are not representative of European soils or conditions (see examples below) also have to be excluded from calculations of variation coefficients, mean / median values and percentiles. A justification for exclusion has to be provided.

A sensible approach should be followed when excluding studies and reliable justification has to be given. Exclusion(s) could be justified in case of the following test conditions (assumption that those conditions have a clear influence on the DT50 and are not relevant for the intended use):

- Tests conducted on soils with very high organic carbon (e.g. peat soils) or with volcanic ash soils; or with agricultural soils not from temperate regions
- Significant overdosing of the test substance;
- Strong decline of microbial activity in laboratory tests during the test period.
- In case of doubt whether a value should or should not be excluded from further consideration, a consultation with the competent authorities is recommended.

### 8.1.3  Criteria to accept field studies

Field studies should be based on BBA Guidance (BBA-Guideline IV 4-1 level 2 (1986)), SE-TAC (1995), NAFTA Guidance (2006), USEPA Guideline (2008) or EFSA Guidance (2010) and have to be conducted on arable land and agricultural soils. Extreme locations with respect to soil type and climate (e.g. tropical or boreal locations) must be excluded.

Furthermore, field studies have to be evaluated according to the checklist of the Dutch regulatory authority CTgB as outlined in FOCUS kinetics (FOCUS, 2006). The criteria are summarised in Appendix 1. Depending on the evaluation result a decision is possible whether the field degradation rates and the respective DT50 values can be used for the assessment of the environmental behaviour of an active substance and its relevant metabolites. The criteria are designed to ensure that the field study is adequately performed including sampling and analysis and that the results are critically evaluated with regard to whether processes other than degradation can be neglected.

### 8.1.4  Reference conditions

#### 8.1.4.1  Reference temperature and reference temperature correction

The laboratory DT50 values have to be normalised to a reference temperature of 20 °C if the test was conducted under an incubation temperature other than 20 °C. The normalisation should be based on the recommended default value for the Q10 factor of 2.58 (EFSA, 2008).

The field DT50 values should be normalised to a reference temperature of 20 °C by normalising each single measurement based on measured daily soil temperature or on corresponding air temperature, respectively. Details on the normalisation procedure are described by Michalski et al. (2004a) and FOCUS (2006).

#### 8.1.4.2  Reference moisture and moisture correction

The laboratory DT50 values have to be normalised to a reference moisture content corresponding to a soil water tension of 10 kPa (pF2) based on measured soil water retention values. The normalisation can be based on default values FOCUS (2000) if soil moisture values at pF2 are not experimentally determined for the specific soils. Normalisation is based on the Walker equation with a default value for the moisture exponent of 0.7.

The field DT50 values should be also normalised to a reference moisture content of 10 kPa (pF2) if measured soil moisture values for pF2 are available. If measured soil moisture values are not available, pedotransfer functions (e.g. HYPRES, ROSETTA or other appropriate methods) can be used to estimate the soil water retention characteristics.

Non moisture normalised field DT50 values could also be used as reliable inputs for modelling, because non moisture normalised DT50s measured under field conditions are usually longer than normalised degradation values in relation to pF2 (FOCUS 2006).

### 8.1.5  Metabolites and metabolite scheme

Route and rate of degradation of active substances and their relevant metabolites are important parameters to perform a reliable groundwater simulation. Primary (formed from the active substance directly) and secondary metabolites (formed from a metabolite) have to be considered in the assessment. See FOCUS (2006) for guidance on the estimation of formation fractions (ff) of metabolites and appropriate implementation of metabolism schemes for simulation.

The degradation of an active substance may follow complex pathway schemes. Figure 2 presents the general principle of the degradation of a substance to its degradation products. The substance can either be the parent substance but also be a metabolite. A complex simu-

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lation scheme could be consisting of more than one precursor $i$ when a resulting degradation product degrades further to degradation products different to $CO_2$. For a given number of the precursor $i$ (and i >1) the first precursor 1 would represent the active substance. For i >1 the precursor would represent a metabolite that degrades further to other degradation products. Possible degradation products are metabolites and/or $CO_2$ & bound residues.
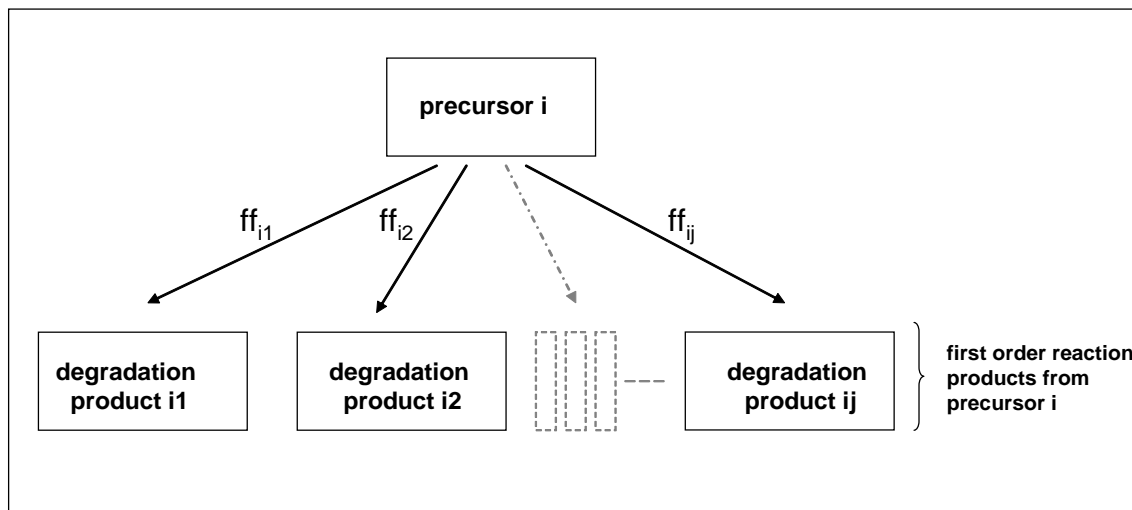


**Figure 2: General principle of degradation of a substance**

In a simulation scheme where more than one metabolite may be formed in parallel (j > 1) the sum of the formation fractions ffij of all degradation products of the respective order i should not exceed 1. If robust formation fractions can only be derived for parts of the pathway (some metabolites), the worst case for the remainder (other metabolites) could be derived by inverse calculations taking into account their formation of robust fits. For a given precursor with **i** and **j = 1,n** the formation fraction can be calculated as follows:


## $\sum$ unknown ff$_{ij}$=1 - $\sum$ known ff$_{ij}$


**Parameter selection for ffij:**

If 3 or more values for formation fractions are available for a respective pathway ffij (i.e. degradation of an active substance to a primary metabolite) and the coefficient of variation (CV) is lower than 100 % the arithmetic mean must be used for simulations. The maximum must be used if less than 3 values are available. If the CV is equal to or higher than 100 % the 90th percentile should be used as a realistic worse case.

If no data are available regarding formation fractions for secondary metabolites (i = 1 and j $\geq$ 1) a value of 1 has to be used. That means the formation fraction for formation of primary metabolite(s) from the active substance and to sink has to be used as described above. The secondary metabolite is formed to 100 % (ff = 1) from the primary metabolite. If the ff for the formation of the secondary metabolite out of the primary metabolite was determined this ff can be used in simulations, too considering the molecular weight and the formation of the primary metabolite.

## 8.2 Selection of half-lives from laboratory and field studies

### 8.2.1 Consideration of high parameter variability for selection of endpoints for modelling

The variability of all DT50 values from laboratory or field studies has to be taken into account for the selection of endpoints for modelling. The coefficient of variation (ratio between standard deviation and arithmetic mean), that presupposes a normal distribution of all values, represents an appropriate statistical parameter to describe the distribution of all individual values around the mean value[2]. With reference to FOCUS (2000) and Michalski et al. (2004a) a coefficient of variation of 100 % is defined as trigger for a high variance.

If the trigger is exceeded and a high variance exists, the 90th percentile of all DT50 values is used for PEC calculations of the parent compound. An additional simulation run using the 10th percentile of the parent DT50 has to be performed to estimate the PEC for the metabolite, whereas degradation values and metabolite formation from other routes remain unchanged.

### 8.2.2 Stepwise procedure regarding non dissociating vs. dissociating substances

A stepwise procedure is recommended to select degradation endpoints for realistic worst case groundwater modelling considering a relationship between degradation behaviour and soil properties, e.g. pH-values, and considering parameter variability.

The decision scheme for the selection of DT50 to calculate groundwater concentrations is provided in Appendix 2.

As a first step, non-dissociating substances are differentiated from dissociating substances that have pKa-values in the pH-range of agricultural soils.

#### 8.2.2.1 DT50 values of non dissociating substances

If the number of available normalised DT50 values of a non-dissociation substance is sufficient (≥ 4 for an active substance and ≥ 3 for metabolites) and the coefficient of variation (CV) of the dataset (based on the ratio of the arithmetic mean and standard deviation) is ≤ 100 %, the geometric mean DT50 value should be used for simulation runs.

In cases where CV is > 100 % it has to be checked whether there is a significant correlation between DT50 values and soil pH.

- If there is no significant correlation, the 90th percentile of DT50 values should be used to model the PECgw for parent. The 10th percentile of DT50 values should be used to model the PECgw for metabolites. Any PEC groundwater calculations for undissociating substances should be performed with the Hamburg reference scenario.

- If there is a significant correlation than the following is to be considered
    o If the substance degrades slower in acidic soils, then the geometric mean of the DT50 values in acidic soils should be used together with the Hamburg scenario.

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[2] For reasons of consistency to previous procedures the CV as the ratio of the arithmetic standard deviation to the arithmetic mean is chosen.

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<ul>
<li>o If the substance degrades slower in neutral and alkaline soils then 2 simulations should be performed (with Kremsmünster and with Hamburg scenario).
<ul>
<li>▪ The geometric mean of the DT50 values in neutral and alkaline soils should be used together with the Kremsmünster scenario.</li>
<li>▪ The geometric mean of the DT50 values in all soils should be used together with the Hamburg scenario.</li>
<li>▪ The worst case result of the 2 scenarios will be compared to the regulatory triggers (see also Appendix 2)</li>
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</li>
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### 8.2.2.2 DT50 values of dissociating substances

For dissociating substances it must be checked whether there is a significant correlation between DT50 values and soil pH. In cases where no correlation exists the same procedure as for non dissociating substances should be used.

If there is evidence for a pH-dependency it should be checked in which way pH-dependency can influence the degradation behaviour.

<ul>
<li>- If the substance degrades slower in acidic soils then the geometric mean of the DT50 values in acidic soils should be used together with the Hamburg scenario</li>
<li>- If the substance degrades slower in neutral and alkaline soils then 2 simulations should be performed (with Kremsmünster and with Hamburg scenario).
<ul>
<li>o The geometric mean of the DT50 values in neutral and alkaline soils should be used together with the Kremsmünster scenario.</li>
<li>o The geometric mean of the DT50 values in all soils should be used together with the Hamburg scenario.</li>
<li>o The worst case result of the 2 scenarios will be compared to the regulatory triggers (see also Appendix 2)</li>
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## 8.3 Selection of adsorption values for modelling

### 8.3.1 General aspects

A precondition for the assessment described below is the availability of adsorption data of an active substance from at least 4 soils (metabolite(s): at least 3 soils) covering a range of different soil properties (texture class, organic carbon content and pH) with an organic carbon content ≥ 0.3 % that have been determined according to OECD Test Guideline 106 (OECD, 1997). Otherwise, adsorption data from a soil that will result in the most conservative estimate of an active substance concentration in the groundwater must be used.

A stepwise procedure is recommended to select sorption endpoints for realistic worst case groundwater modelling considering a relationship between sorption behaviour and soil properties e.g. organic carbon content, pH, cation exchange capacity and considering parameter variability.

The significance of a correlation between Kf-values and soil properties has to be investigated with the Kendall rank correlation test, which is implemented in the 'Excel'-tool 'Input-Decision 3' (see chapter 7).

In order to obtain meaningful averages of sorption values from different soils a correlation between sorption and e.g. pH has to be investigated. Such a correlation is most likely for

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[3] Current version will be "Input decision 3.0"

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dissociating substances. Therefore, non-dissociating and dissociating substances must be distinguished in a first step. Only those substances with pKa-values in the range of the pH-values of the agricultural soils of interest must be considered.

The decision tree is given in Appendix .

### 8.3.2 Stepwise procedure for non-dissociating substances

#### 8.3.2.1 Correlation between Kf-values and organic carbon content (Corg)

If for a non-dissociating substance a significant correlation between Kfoc and organic carbon content is established the arithmetic means of the Kfoc values and Freundlich exponents (1/n) of all soils are used as input parameters for a simulation model[4].

#### 8.3.2.2 Variation coefficient (CV) of Kfoc-values ≤ 60 %

If there is no significant correlation between Kf-values and organic carbon content, but the coefficient of variation of the Kfoc-values is ≤ 60 % the arithmetic means of the Kfoc-values and of the Freundlich exponents (1/n) of all soils can be used for the simulation model.

#### 8.3.2.3 Correlation between Kf-values and other soil properties (pH, clay, cation exchange capacity (CEC)

If there is no significant correlation between Kf-values and organic carbon content and the coefficient of variation related to the arithmetic mean of the Kfoc-values is more than 60 %, the correlation of the Kf-values to other soil properties such as pH, clay content, and cation exchange capacity should be checked.

If the correlation of a Kf-value with any other soil parameter (clay, CEC, pH) is significantly higher than its correlation with organic carbon content the use of the Kfoc-value is not appropriate. Horizon-specific Kf-values have to be used in this case[5].

Note: Generally, the use of horizon-specific Kf-values is limited to horizons containing sorptive particles like organic carbon, clay or sesquioxides. Kf-values should be set to zero for horizons without sorptive particles.

#### Correlation between Kf and pH

In case of a significant correlation between Kf-values and pH, the stepwise scheme for dissociating substances must be used and scenario specific Kf-values should be determined for both the Hamburg and Kremsmünster scenario.

#### Correlation between Kf and clay or cation exchange capacity (CEC)

In cases where no significant correlation between Kf-values and % organic carbon content or pH of the soils can be observed, relationships between Kf-values and clay or CEC of the soils have to be checked.

If Kf-values correlate with the clay content and / or the CEC of the soil the Kf-values have to be determined for each horizon of the Hamburg soil reference scenario by means of the respective regression equation.

If correlation of both parameters (clay and CEC) is significant, the parameter with the strongest correlation for calculating horizon specific Kf-values should be selected or in most cases

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[4] e.g. activation of the "Kf-value - calculated with Kfoc" function in FOCUS PELMO

[5] e.g. activation of the "Kf-value - direct input" function in FOCUS PELMO

a multiple regression is the better choice to estimate the horizon specific parameters. For the Freundlich exponent (1/n) the arithmetic mean calculated from values of all soils has to be used. Calculations have to be done with Hamburg scenario, only.

In the FOCUS (2009) report CEC-values for the FOCUS Hamburg[6] and Kremsmünster scenarios are not provided. The CEC is essentially a function of two soil properties, the clay content and its OC-value (Schachtschabel et al. 1989, Krogh et al. 2000). Therefore it is proposed to use the pedotransfer function given in the German soil survey guide (AG-Boden, 2005) to calculate CEC-values for Hamburg and Kremsmünster the CEC in mEq $(100 \text{ g})^{-1}$ can be written as

CEC = 0.5 Clay $(g (100 \text{ g})^{-1})$ + 0.05 Silt $(g (100 \text{ g})^{-1})$ + 2 $f_{OC}$ OC $(g (100 \text{ g})^{-1})$. Note: $f_{OC}$ is the mass ratio between soil organic matter and carbon that was set to $f_{OC}$= 1.724.

### 8.3.2.4 Multicorrelation

Generally, if there is no correlation between Kf-values and other soil parameters, it has to be checked whether a significant correlation can be demonstrated by the exclusion of outlier values or any other considerations for relevant soil parameters.

If a good individual correlation cannot be found, the presence of a correlation between Kf and several soil properties (multiple correlations) should be considered. Depending on the correlation, appropriate values should be determined specific to the particular horizon by means of the specific regression equation and the properties of the Hamburg soil[7].

## 8.3.3 Stepwise procedure for dissociating substances

### 8.3.3.1 Correlation between Kfoc-values and pH for dissociating substances

If there is a significant correlation between Kfoc-values of dissociating substances and pH, the pH-tools "pH-dependent sorption" in the model should be used.

With respect to the parameterisation, refer to FOCUS (2009) and to the manuals of the FOCUS model.

For the Freundlich exponent (1/n) the arithmetic mean of all soils should be used. To determine a realistic worst case for the PECgw, simulations have to be run with the Hamburg reference scenario representing acidic soils and with the Kremsmünster reference scenario representing neutral/alkaline soils.

According to FOCUS (2009) the measured relationship between Kfoc and pH must be consistent with the FOCUS leaching scenarios that are parameterised with pH-values according to pH-$H_2O$[8]

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[6] Measured CEC-values for Hamburg soil scenario given by Michalski et al. (2004a)

[7] scenario "Kf-value - direct input" in FOCUS PELMO 4.4.3

[8] If the soil pH-H2O is not indicated in the available adsorption studies, it can be calculated according to FOCUS (2009) as follows:
pH-H2O = 0.820 pH-KCl + 1.69
pH-H2O = 0.953 pH-CaCl2 + 0.85

where pH-KCl is the pH measured in an aqueous solution of 1 mol/L of KCl and where pH-CaCl2 is the pH measured in an aqueous solution of 0.01 mol/L of CaCl2

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### 8.3.3.2 Correlation between Kf-values and pH

If there is no correlation between Kfoc-values and pH the possibility of a correlation between Kf-values and pH has to be checked according to the procedure described in chapter 7 (see Kendall test). If a correlation between Kf-values and pH is established, scenario specific Kf-values for the Hamburg and Kremsmünster reference scenarios have to be estimated.

Generally the use of the estimated scenario specific Kf-values is limited to horizons which contain sorptive particles like organic carbon or clay or Fe- / Al-oxides. Kf-values are set to zero for horizons without sorptive particles.

− **Negative correlation**

For acidic substances with a significant negative correlation between Kf-values and pH, two simulation runs have to be performed. The Kremsmünster reference scenario is used in a first step with the Hamburg reference scenario used in a second step.

For calculations with the Kremsmünster reference scenario the arithmetic means of the Kf-values and Freundlich exponents (1/n) of soils under neutral and alkaline conditions should be selected. If possible, the selection should be related to pH-$H_2O$ values that are approximately > 1 to 2 units higher than the pKa-value of the substance. If the pKa is < 5, kf-values mainly from neutral and alkaline soils but also slightly acidic soils would be appropriate. Otherwise the 10th percentile of the Kf-values has to be used.

In addition, a simulation run with the Hamburg reference scenario is required using the arithmetic means of the Kf-values and Freundlich exponents (1/n) from all soils.

The highest PECgw value as a result of the two simulation calculations is selected to be the regulatory assessment endpoint.

− **Positive correlation**

If there is a significant positive correlation between Kf-values and pH, the arithmetic means of the Kf-values and the Freundlich exponents (1/n) from calculations using only the acidic soils have to be taken into account. Due to the low pH the Hamburg reference scenario should be used for these simulation calculations as worst case.

### 8.3.3.3 No correlations between Kfoc- or Kf-values and pH

If there is no significant correlation between Kfoc- or Kf-values and pH, other correlations have to be checked and the stepwise scheme as applied for non-dissociating substances should be followed.

### 8.3.4 Other dependencies

### 8.3.4.1 No correlation between Kf-values and any other soil properties

If no significant correlation between Kf and one or more soil properties is found, it is expected that adsorption behaviour does not vary between the particular horizons. In these cases the same Kf-values and Freundlich exponents (1/n) are used for each horizon that contains sorptive particles.

If the coefficient of variation of Kf-values is ≤ 60 % related to the arithmetic mean, the arithmetic mean of the Kf-values of all soils can be used. Otherwise the 10th percentile of the Kf-values must be used. For determination of the Freundlich exponent (1/n) the arithmetic mean of all soils is used.

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### 8.3.4.2 Experimentally determined horizon-specific Kf-values

If the Kf-values are not sufficiently well represented by a correlation equation with several soil properties, experimentally determined horizon-specific Kf-values may be entered. The properties of the soil tested should be in the range of the Hamburg reference soil.

Independent of the stepwise scheme described here, it is always possible to enter experimentally determined horizon-specific Kf-values directly into the model[9]. Note, that these values have to be determined in a soil profile that leads to weak adsorption of the test substance and thus represents a realistic worst case.

### 8.3.5 Choice of Freundlich exponent values (1/n) if only Kd-values are available

According to OECD 106 the equilibrium partition between the bulk soil matrix and the soil solution must be determined in a range of soil solution concentrations to obtain the parameters of the Freundlich isotherm, the Freundlich partition coefficient (Kf) and the Freundlich exponent (1/n) that describes the effect of solution concentration on the partitioning.

According to FOCUS (2000) the Freundlich exponent (1/n) usually ranges between 0.7 and 1.0. Accurate determination of the Freundlich adsorption isotherm is only possible if either the product from multiplying the Kd-value by the soil / solution ratio is > 0.3 (indirect method: measurements are based on concentration decrease in the aqueous phase), or the product is > 0.1 (direct method: both phases are analysed, see OECD guideline 106, p. 12). In cases where a determination of reliable Freundlich exponents according to the OECD guideline 106 (1997) was not possible because of experimental difficulties that could not be overcome (e.g. the active substance was unstable) and a high variation of 1/n-values exists with single values below 0.7 or above 1 for active substances or metabolites, a default value of 0.9 can be used for PEC groundwater estimations[10].

In cases where only measured Kd-values for a single soil solution concentration are available or estimated quantitative structure-activity relationship (QSAR) adsorption values are seen, it is necessary to set the corresponding 1/n-value to 1.

## 8.4 Simultaneous effect of the pH-value on degradation and sorption

Both, the degradation and sorption behaviour of active substances or metabolites in soil might be pH dependent. Additive as well as compensating effects may occur, which must be taken into account when selecting appropriate model inputs.

Parameters should be selected sensible to obtain an overall realistic worst case. Unrealistic parameter combinations have to be avoided. In such cases the conceptual approach has to be explained very clearly in regulatory submissions.

## 8.5 Kinetic sorption

Kinetic or non-equilibrium sorption is a known process and its relevance for the transport behaviour of pesticides has been shown (e.g. Boesten, 1987, Streck et al., 1995).

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[9] activation of the "Kf-value - direct input" function in FOCUS PELMO

[10] EFSA (2010) excerpt from "Data requirements, study guideline, guidance and consensus of member state fate and behaviour experts on soil adsorption measurements and selection of the slope (1/n-value) that describes the Freundlich coefficient. Clarification note from EFSA (PRAPeR unit).

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Experimental studies that demonstrate an increase in pesticide sorption with time may be submitted to regulatory authorities as part of the regulatory data package. The results of these studies are used by applicants as higher tier options to revise estimates of predicted environmental concentrations in groundwater. Pesticide leaching models that include the concept of kinetic sorption are used for this purpose. In FOCUS (2009) it is principally described how to conduct and evaluate those studies and how to include the derived kinetic sorption parameters into the exposure assessment. It is commonly accepted that kinetic sorption parameters can be determined with the help of aged-sorption laboratory experiments. These experiments are similar to OECD Guideline 307 laboratory degradation studies (2002), but modified to include an additional desorption step with $CaCl_2$-solution to estimate the aqueous phase concentration. Some basic information is given in Appendix 4.

It was shown by van Beinum & Beulke (2010) that the derived kinetic sorption parameters used in the leaching models show strong influence on the PECs[11]. Higher tier groundwater simulations including kinetic sorption should consider the actual draft guidance within the EU (van Beinum & Beulke, 2010). In particular cases, different approaches might be accepted if they are well-founded. Close cooperation between the notifier and the competent authority is necessary when kinetic sorption is being assumed as a relevant process that should be taken into account in the exposure assessment.

The possibility to consider kinetic sorption is given in versions of the FOCUS-models which are updated under FOCUS (2009). In FOCUS PELMO two options are available: the non-equilibrium sorption PEARL approaches (Leistra et al., 2001) as well as the STRECK approach (Streck et al., 1995).

For the PEARL approach the so-called fNE-parameter that is the ratio of non-equilibrium and equilibrium sorption (Kf,oc-neq / Kf,oc-equ) as well as the desorption rate kdes is needed. In the PEARL approach degradation takes only place in the equilibrium phase (liquid phase and equilibrium sorption phase). Therefore specific degradation rates have to be estimated that can be used in combination with kinetic sorption parameters, only.

The Streck approach uses the total sorption that is the sum of non-equilibrium and equilibrium sorption (Kf,oc-tot = Kf,oc-neq + Kf,oc-equ) and the fraction of equilibrium sorption (Kf,oc-equ / Kf,oc-tot) as well as the rate constant alpha. The approaches are mathematically equivalent and can be transferred. A comprehensive overview is given in FOCUS (2009).

## 8.6 Plant uptake

Active substances as well as metabolites in soil can be taken up by plants via the root system. The amount that is taken up is no longer available for leaching processes.

The process of plant uptake is implemented in FOCUS PELMO as well as in other models and depends on climate and crop parameters within the model. The amount of plant uptake is calculated in principle by considering the concentration of a substance in pore water in the plant root zone, the amount of transpiration (i.e. practically the water volume consumed by the plant) and the plant uptake factor (PUF). Here the plant uptake factor represents a simplified transfer coefficient to describe the translocation of substance from pore water to the plant.

Mass of substance in plant (plant uptake) [mg]

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[11] Therefore, CRD started an initiative to develop a more detailed guidance on the exact design and the parameter fitting of laboratory aged sorption studies that is currently under discussion (van Beinum & Beulke, 2010). Some lack of agreement on details still exists regarding how aged sorption studies should be conducted, analysed, interpreted and hence used in regulatory exposure assessments.

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= substance concentration in pore water [mg/L] * amount of transpiration [L] * plant uptake factor [-]

In the FOCUS PELMO model the uptake factor can be defined separately for the active ingredient and metabolite(s). The parameterisation of the plant uptake factor requires data on the uptake of the substance into the whole plant. FOCUS (2000, 2009) refers to the transpiration stream concentration factor (TSCF) as a surrogate parameter estimating plant uptake. In line with the processes actually simulated in PELMO 3.0 the plant uptake factor may be experimentally determined by measuring substance mass and water volume taken up by the plant exposed to hydroponic solutions spiked with the test item. The resulting concentration in the solution taken up by the plant can be related to the substance concentration in the test solution to calculate the PUF. Currently methods are under development how to determine the factor.

For systemic, non ionised compounds FOCUS (2000) recommends the use of a default value for the uptake factor on the basis of the Briggs equation (Briggs et al., 1982) that provides a relationship between TSCF and octanol / water partitioning coefficient (logKow) under specific test conditions. This relationship may not be applicable for all substances, crop combinations or experimental conditions as documented in several studies due to the high variability of uptake factors found for substances having a similar logKow in different crops (Briggs et al., 1982; Hsu et al., 1990; Burken & Schnoor 1998; Dettenmaier et al., 2009). This indicates that the uptake factor is not only characteristic for a substance (logKow, pKa) but also depends on the experimental conditions (duration of exposure, temperature, pH of the pore water and nutrient solution in the experiment, respectively) and the crop (content of lipid, fiber, and carbohydrate of roots and shoots; root system) (Walker, 1973; Simonich and Hites, 1994; Bromilow and Chamberlain, 1995; Hung and Mackay, 1997; Chiou et al., 2001; Collins et al., 2006).

Hence in tier 1 modelling the uptake factor should be set at zero for all substances (active ingredient and metabolites, ionic and non-ionic) in the FOCUS PELMO scenario file (uptake factor=0) in order to simulate a worst case scenario.

In tier 2 modelling the PECgw can be refined by experimental determination of the substance specific plant uptake factor (FOCUS 2009). This approach should be developed in close collaboration between the notifier and the responsible authority[12].

According to FOCUS (2009) plant uptake may be further considered in combination with DT50 values derived from field studies with bare soil but is not possible if field degradation rates derived from trials conducted with crops are used for modelling, unless it can be demonstrated that plant uptake in the cropped study did not play a significant role[13].


## 8.7   Crop rotation

Simulation of a crop rotation may be relevant for active substances and / or metabolites from plant protection products to enable the substance to pass the regulatory limit values, in the

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[12] Presently, for ionic and nonionic substances there is neither a standardised method nor an agreed guideline for the measurement of an uptake factor available. A standard approach to quantify the uptake factor with laboratory tests is currently under development. Here the factors influencing the plant uptake should be clarified in more detail to possibly conclude general approaches to deduce defaults for uptake factors or test designs for particular substances and/or crop combinations if applicable.


[13] This may be demonstrated by modelling or by logical conclusions e.g. if soil was sampled between rows that were insignificantly influenced by crop roots

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case where they would not pass with yearly applications and the interval between two applications needs to be increased. However, all substances should first be tested in monocropping application regimes, as described below in more detail.

According to FOCUS (2009) a yearly application of the active substance in combination with monocropping over a time period of 26 years (including a warming up period of 6 years) should be always used in the groundwater model at tier 1 (see Table 1).

In agricultural practice some crops like wheat and maize can be cultivated on the same field one year after another without effects on crop yields. Hence, the same active substance could be applied on the same agricultural field every year.

Other crops are not cultivated on the same agricultural field every year due to phytosanitary reasons. Cultivations with shorter time intervals for such crops would lead to depressions of harvest due to increased pest pressure from nematodes or soil borne fungal diseases. Therefore, crop rotation is usually maintained as good agricultural practice. A treatment with the same active substance every year on the same field could be certainly excluded if the active substance is especially designed for the use in one of these rotational crops, only (e.g. potatoes). Otherwise, a treatment of the same active substance with different application rates and application times in several subsequent years on the same field must be expected even for these crops, because plant protection products with the same active substance can be on the market for other crops which might be cultivated in the same rotation.

Recommendations are given below on how to implement crop rotation in tier 2 groundwater simulations and risk management for substances submitted for crops which are usually cultivated in rotation (e.g. potatoes, sugar and fodder beets, winter rape, peas, beans, cabbage), and in cases where the predicted environmental concentration in groundwater at tier 1 exceeds the obligatory trigger values. It is not intended to implement realistic perennial crop rotation patterns in groundwater simulations at tier 2, because cultivation practices in different regions and farms can highly differ. Examples for crop rotations common in agriculture in Germany are presented in Appendix 5. However, the consequential complexity of possible crop combinations and application pattern over several years may complicate the identification of an appropriate realistic worst case scenario for groundwater risk assessment. In addition, the original FOCUS input files cannot be used for such simulations.

As a consequence, in tier 2 simulations it is recommended to gradually extend the system of annual application if crop rotation is well-founded for the intended crop (see Table 1, available rotations in Appendix 5). Even if it is known that the submitted crop is usually cultivated only every three years (e.g. potatoes) an additional simulation should be run first for 46 years including a warming up period of 6 years according to FOCUS (2009). In this simulation an application of the active substance should be conducted every second year. The crop is considered as monocropping over the whole simulation period. If the predicted environmental concentration in groundwater still exceeds the relevant trigger values, a further simulation should be run for 66 years, at which an application of the active substance every third year is conducted and the crop is again grown as permanent crop in the model.

Depending on the results of the simulations, the authorisation of the plant protection product may be only granted in Germany with the restriction to apply on the same field only every second or third year, respectively, in order to guarantee the necessary minimum time interval between two applications for the purpose of groundwater protection.

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**Table 1: Parametrisation of tier 2 groundwater simulations considering crop rotation for potatoes, sugar and fodder beets, winter rape, legume (peas, beans) and cabbage**

| | tier 1 | | tier 2 Step 1 | | tier 2 Step 2 | |
|---|---|---|---|---|---|---|
| Application pattern of soil relevant application amount | Every year | | Every second year | | Every third year | |
| Simulations period (6 years of warming up period included) | 26 years | | 46 years | | 66 years | |
| Crop setting | Monocropping | | Monocropping | | Monocropping | |
| **Examples of simulation runs** | | | | | | |
| year 1 | 1kg as/ha / potatoes | | 1kg as/ha / potatoes | | 1kg as/ha / potatoes | |
| year 2 | 1 kg as/ha / potatoes | | 0 kg as/ha / potatoes | | 0 kg as/ha / potatoes | |
| year 3 | 1 kg as/ha / potatoes | | 1 kg as/ha / potatoes | | 0 kg as/ha / potatoes | |
| year 4 | 1 kg as/ha / potatoes | | 0 kg as/ha / potatoes | | 1 kg as/ha / potatoes | |
| year 5 | 1 kg as/ha / potatoes | | 1 kg as/ha / potatoes | | 0 kg as/ha / potatoes | |
| year 6 … | 1 kg as/ha / potatoes … | | 0 kg as/ha / potatoes … | | 0 kg as/ha / potatoes … | |
| Simulation result depending on obligatory trigger values, e.g. 0.1 µg/L | PECgw < trigger | PECgw > trigger | PECgw < trigger | PECgw > trigger | PECgw < trigger | PECgw > trigger |
| Authorisation possible / restrictions | Yes/ No restriction | No/ Check possibility for Tier 2 calculation step 1 | Yes / Application restrictions for plant protection products with the same active substance on the same field every second year | No/ Check possibility for tier 2 calculation step 2 | Yes/ Application restrictions for plant protection products with the same active substance on the same field every third year | No |

# 9 Other input parameters

## 9.1 Application rates and date of application

The data of application must be entered according to Good Agriculture Practice (GAP). Considering to the crop development stages (BBCH codes) and the corresponding interception those application rates should be used that lead to the highest soil load. A conservative selection of different application amounts and different application rates in combination with the cultivation of different crops might be necessary in tier 2 simulations considering crop rotation in the modelling.

The program AppDate (Klein, 2007) can be used to determine application dates for the scenario Hamburg with respect to crop development stages (BBCH codes). Application dates can also be estimated based on phenological stages of crops as e.g. described by Gericke et al. (2010). Alternatively application dates from residue trials, that are submitted in the 'residue section', can be used.

## 9.2 Crop interception

Interception and hence effective soil load rates are calculated according to the recommendations of the FOCUS generic guidance paper (2002). The actual amount of active substance reaching soil is derived from the maximum application rate reduced by crop interception if plants are present at the time of application. Crop development stages (BBCH codes) with the corresponding interception values based on the FOCUS recommendations can also be obtained with the program AppDate (Klein, 2007). In cases, where no information about interception are given in the FOCUS generic guidance paper (2002), e.g. vegetables, conservative assumed interception values as recommended for Step 2 calculations in the FOCUS Surface water report (2002) can be applied.

## 9.3 Soil

The FOCUS soil scenarios Hamburg and Kremsmünster (FOCUS 2009) are used for selecting model input values, dissipation and sorption depending on the decision scheme charts in this paper (see Appendix 3: Adsorption Decision Scheme for PECgw and Appendix 3). The Hamburg and Kremsmünster reference soil profile is used down to a depth of 1 m with the biodegradation factors given in the FOCUS PELMO 4 manual (Klein, 2011).

## 9.4 Simulation period

A simulation period of 26 years is normally used, including a 6 year warming up period (FOCUS, 2009). When the substance is applied every second or every third year (if crop rotation is considered) the simulation period will be extended up to 46 or 66 years, respectively (FOCUS, 2009).  See section 8.7 .

## 9.5 Climate

For the simulation runs the FOCUS (2009) climate scenarios for Hamburg and Kremsmünster are used. Further information about the climate data files are given in the FOCUS report (2000, 2009).

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## 9.6 Erosion, runoff, volatilisation

These processes are not accounted for in the simulations. The corresponding submodules should be deactivated. The model should only simulate degradation, sorption and leaching of the substance(s) reaching the soil surface. If measured DegT50 are available the vapour pressure should be taken into account.

## 9.7 Soil photolysis

In general this process is not accounted for the simulation. Please contact the responsible authority in special cases.

## 10 Assessment of simulation results

The simulation calculates substance concentrations in accordance with the FOCUS procedures (mass leached divided by water volume leached) over simulation periods of 26, 46 and 66 years depending on treatment and crop rotations. Main simulation results are the average concentrations of the active substance and/or metabolite(s) in the leachate (in µg/L) at a depth of 1 m. The 80th percentile average concentration over the FOCUS period is selected as the critical endpoint of the assessment (the first six years as "warming up period" are excluded). This value represents the individual PECgw for each compound (predicted for an overall 90th percentile worst case scenario setting). In case that the simulation-based PECgw of the active substance (or for a relevant metabolite) exceeds 0.1 µg/L, a higher tier study or refinement is required. For non relevant metabolites in accordance with Sanco/221/2000 -rev.10- final the threshold of concern approach of 0.75 and 10 µg/L respectively has to be considered in the exposure assessment.

## 11 Outlook

The realisation of the recent FOCUS (2009) recommendations for higher tier leaching assessments (Figure 1, higher tier modelling and higher tier outdoor studies, tier 3 & 4,) is currently under internal discussion within the regulatory authorities. Publication of a finalised opinion of the German regulatory authorities on this part of the tiered assessment is planned in near future.

Some older guidance on conducting studies already exist on national level in various EU member states and in released opinions, e.g. on outdoor lysimeter studies and on groundwater monitoring studies. Such guidance was also published on German national level.

Therefore each applicant who comes to the conclusion that, based on the modelling results, a higher tier study is needed for a successful regulatory submission, is hereby strongly advised to discuss the case specific approach which should be taken with the competent authorities in advance of any submission. Consultation with the competent authorities is also recommended in specific or borderline case, since it is impossible to cover every possible case within the scope of such a publication.

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FOCUS PELMO 4 Input Parameters

# 13 Appendixes

## Appendix 1: CTgB criteria as outlined in FOCUS kinetics (FOCUS, 2006)

- Check that only a non-significant fraction of the dose can have leached out of the soil layers that were sampled (consider the amount of rainfall and concentration measured in the deepest sampled layer);
- Check that only a non-significant fraction of the dose disappeared via processes at the soil surface such as volatilisation or photochemical transformation (consider the period between spraying and the first significant rainfall event; check additionally that there is no initial fast decline followed by a slower decline; a recovery in the field that is much lower than the dose is also an indication of losses at the soil surface);
- Check that the decrease of the total amount with time corresponds reasonably well with first-order kinetics (either via curve-fitting or via applying a simulation model). Calculation procedure according to FOCUS degradation if there is much scatter in the relationship between total amount and time (probably due to an inadequate sampling strategy) this should be taken into account in the interpretation; estimation of a transformation rate in soil may not be acceptable;
- Check whether the soil has been characterised (organic matter, clay etc.);
- Check whether the location can be considered representative with respect to soil type and climate;
- Check whether meteorological data are available at least for the duration of the field experiment, and whether a correction for the difference between the actual soil temperature (mean temperature measured during the day in top soil layer) and 20°C has been made (FOCUS, 2000). An acceptable alternative is air temperature during the day measured on site or at a nearby weather station. The soil temperature can be calculated based on air temperature;
- Check whether the dose is reported and whether the formulated product is relevant (no granulate or slow release);
- If inverse modelling was used, check whether the model used is acceptable. The calculation procedure should be according to FOCUS (2006);
- Check whether analytical procedure was documented well and whether recovery was acceptable;
- Check history of pesticide use on plot. No active ingredient or chemical analogue should have been used in preceding years;
- Check method of application. Pesticide should not be applied below soil surface;
- Check method of sampling. Method of sampling should be adequate;
- Check influence of crop. Uptake of pesticide by crop should be negligible and taken into account in the interpretation.

# Appendix 2: Selection of DT50 Decision Scheme for PECgw

Are studies with less then 4 soils for the active substance and 3 soils for the metabolites available?

**yes** →

**Hamburg scenario:**
Maximum of the $DT_{50}$ values
**or**
**demand for a study with the required number of soils**

**no** ↓

Is it a dissociating substance?

**yes** →

Does a significant correlation between $DT_{50}$ and pH-value exist?

**yes** →

How to consider the pH-dependency of the degradation behaviour in the PEC calculation?

**no** ↓ (dissociating substance)

**no** (correlation) →

Is the CV of the $DT_{50}$ values ≤ 100 %?

**yes** →

**Hamburg scenario:**
Geometric mean of the $DT_{50}$ values from all soils

**no** ↓

Does a significant correlation between $DT_{50}$ and pH-value exist?

**yes** →

**no** ↓

**Hamburg scenario:**
90/10th percentile of the $DT_{50}$ values of active substance to calculate PECs for active substance/ metabolites

Substance degradates slower in acidic than in alkaline soils

**Hamburg scenario (pH-value 6.4-5.5):**
Geometric mean of the $DT_{50}$ values of the acidic soils

Substance degradates slower in alkaline than in acidic soils

**2 simulations and selection of the worst case PECgw**

**1.simulation with Kremsmünster scenario (pH-value 7.7-7.0):**
Geometric mean of the $DT_{50}$ values of the neutral and alkaline soils

**2.simulation with Hamburg scenario (pH-value 5.5-6.4):**
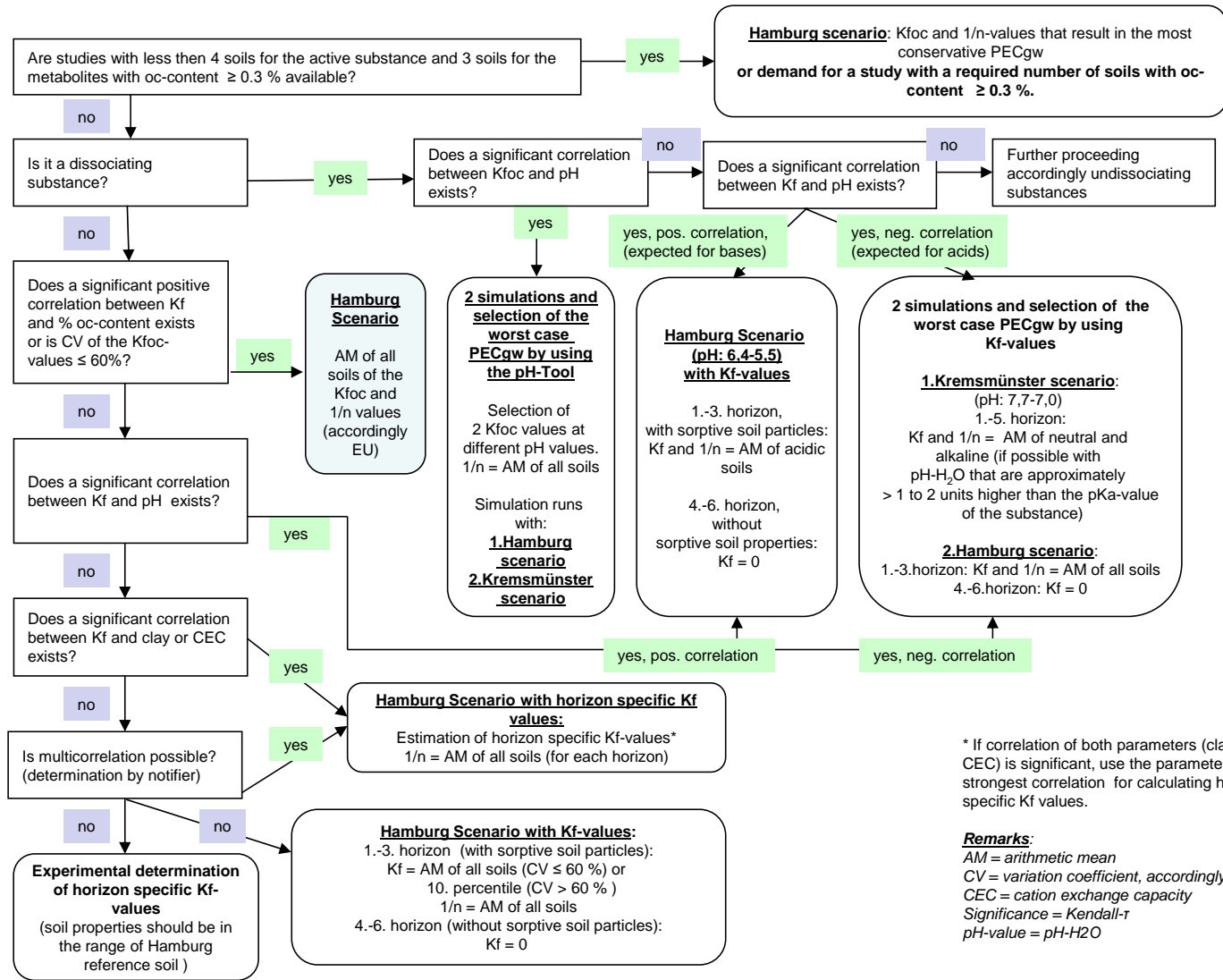Geometric mean of the $DT_{50}$ values from all soils

**Remarks:**
*CV = coefficient of variation (standard deviation divided by arithmetic mean)*
*Significance = Kendall-τ*

FOCUS PELMO 4 Input Parameters

# Appendix 3: Adsorption Decision Scheme for PECgw

**Are studies with less then 4 soils for the active substance and 3 soils for the metabolites with oc-content ≥ 0.3 % available?**

yes →

**Hamburg scenario**: Kfoc and 1/n-values that result in the most conservative PECgw
**or demand for a study with a required number of soils with oc-content ≥ 0.3 %.**

no ↓

**Is it a dissociating substance?**

yes → **Does a significant correlation between Kfoc and pH exists?**

no → **Does a significant correlation between Kf and pH exists?**

no → **Further proceeding accordingly undissociating substances**

no ↓

**Does a significant positive correlation between Kf and % oc-content exists or is CV of the Kfoc-values ≤ 60%?**

yes →

**Hamburg Scenario**

AM of all soils of the Kfoc and 1/n values (accordingly EU)

yes, pos. correlation, (expected for bases)

yes, neg. correlation (expected for acids)

yes ↓ (from Kfoc and pH)

**2 simulations and selection of the worst case PECgw by using the pH-Tool**

Selection of 2 Kfoc values at different pH values. 1/n = AM of all soils

Simulation runs with:
**1. Hamburg scenario**
**2. Kremsmünster scenario**

**Hamburg Scenario (pH: 6,4-5.5) with Kf-values**

1.-3. horizon, with sorptive soil particles: Kf and 1/n = AM of acidic soils

4.-6. horizon, without sorptive soil properties: Kf = 0

**2 simulations and selection of the worst case PECgw by using Kf-values**

**1. Kremsmünster scenario**:
(pH: 7,7-7,0)
1.-5. horizon:
Kf and 1/n = AM of neutral and alkaline (if possible with pH-H₂O that are approximately > 1 to 2 units higher than the pKa-value of the substance)

**2. Hamburg scenario**:
1.-3.horizon: Kf and 1/n = AM of all soils
4.-6.horizon: Kf = 0

no ↓

**Does a significant correlation between Kf and pH exists?**

yes →

no ↓

**Does a significant correlation between Kf and clay or CEC exists?**

yes, pos. correlation

yes, neg. correlation

yes →

**Hamburg Scenario with horizon specific Kf values:**
Estimation of horizon specific Kf-values*
1/n = AM of all soils (for each horizon)

no ↓

**Is multicorrelation possible? (determination by notifier)**

yes →

no ↓        no →

**Experimental determination of horizon specific Kf-values**
(soil properties should be in the range of Hamburg reference soil )

**Hamburg Scenario with Kf-values:**
1.-3. horizon (with sorptive soil particles): Kf = AM of all soils (CV ≤ 60 %) or 10. percentile (CV > 60 % ) 1/n = AM of all soils
4.-6. horizon (without sorptive soil particles): Kf = 0

\* If correlation of both parameters (clay and CEC) is significant, use the parameter with the strongest correlation for calculating horizon specific Kf values.

***Remarks***:
*AM = arithmetic mean*
*CV = variation coefficient, accordingly AM*
*CEC = cation exchange capacity*
*Significance = Kendall-τ*
*pH-value = pH-H2O*

## Appendix 4: Basic Information on Kinetic Sorption Process

The kinetic-sorption model according to Boesten et al. (1989) discussed here considers 3 phases, the dissolved phase (Cw), the equilibrium sorbed phase (Cs eq) and the non-equilibrium sorbed phase (Cs neq) of a compound in a soil system (see Figure 3). The degradation rate in the equilibrium domain (kt), the desorption rate constant (kd) the ratio of non-equilibrium domain to equilibrium domain (fne), and the initial value ot the equilibrium sorbed concentration Cs eq 0 are important parameters.

Kd, Kf neq, 1/n

Cw ↔ Cs eq

Kf eq, 1/n

kt    kt

Cs neq

equilibrium domain                    non-equilibrium domain
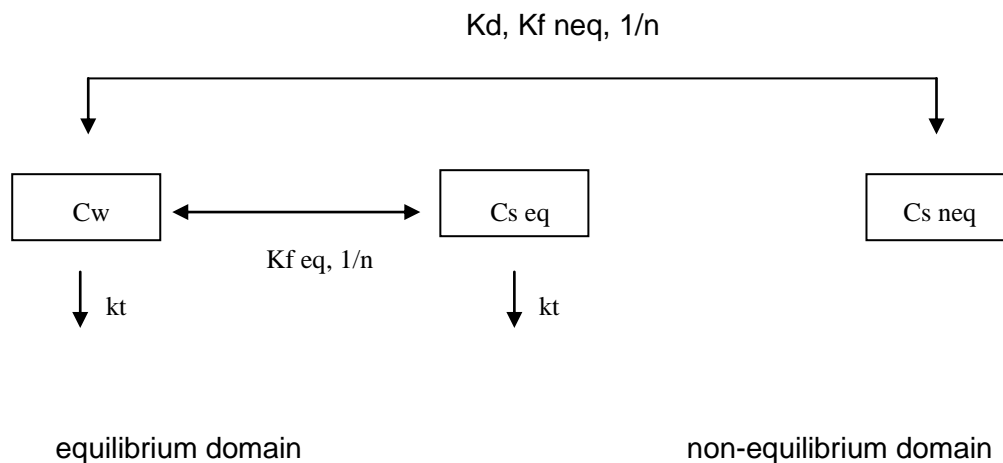
**Figure 3: 3-compartment sorption kinetic model (Beulke & van Beinum, 2010; Sur et al., 2009)**

It is normally assumed that the sorption of a compound to soil is an instantaneous process leading to an equilibrium between the dissolved and the sorbed phase. While this is an appropriate description for a number of compounds there are others whose behavior is characterized by kinetically controlled sorption processes. If only the standard batch equilibrium experiment is applied to such compounds the kinetically controlled part of their sorption potential is neglected. Consequently the mid- and long-term sorption is underestimated and the mobility is overestimated. This is of particular importance for the realistic prediction of the leaching behavior.

The relation between dissolved and equilibrium sorbed phase is characterized by instantaneous equilibrium between the concentrations in both phases and is described by the Freundlich isotherm as:

$$Cs_{eq} = Kf_{eq} \times C_w^{1/n}$$

$Cs_{eq}$    concentration in the equilibrium sorbed phase, in mg / Kg dry soil,
$C_w$       concentration in the dissolved phase, in mg/L water,
$Kf_{eq}$    Freundlich distribution coefficient for equilibrium domain, in L / Kg,
$1/n$       Freundlich exponent.

(Atkins et al. 2004; Klöpffer, 1996)

The concentration in the non-equilibrium phase Cs neq is defined as the non-equilibrium sorbed mass of a substance / mass of dry soil. It is related to Cs eq by first-order kinetic exchange defined as

$$\frac{d\,Cs_{neq}}{dt} = Kd \; x \left[ \; \frac{Kf_{neq}}{Kf_{eq}} \; x \; Cs_{eq} \; - \; Cs_{neq} \; \right]$$
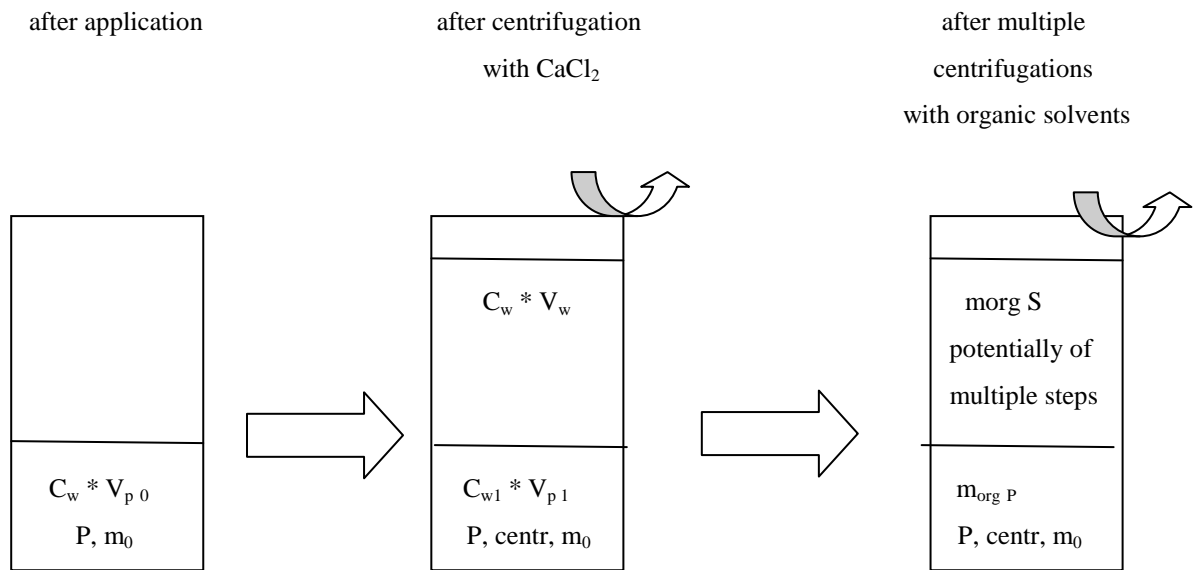
> Kd         : kinetic-sorption rate constant
> Kf $_{neq}$    : Freundlich coefficient for the non-equilibrium domain.

The Freundlich exponent 1/n is assumed to be equally valid for the equilibrium and non-equilibrium domain.

At time of application, the non-equilibrium domain is empty, that is $Cs_{neq}$ (t = 0) = 0 by definition, where t is the time after application. The flux into the non-equilibrium phase is driven by the difference between actual and infinite value, with maximum flux when $Cs_{neq}$ (t = 0) = 0. After a sufficient period of time $Cs_{neq}$ has reached a constant value, i.e. $dCs_{neq}$ / dt = 0, that depends mainly on the ratio between the Freundlich coefficients $f_{ne}$ = $Kf_{neq}$ / $Kf_{eq}$. If the dissolved and equilibrium sorbed phase is rapidly removed or changed by e.g. decanting of a supernatant in a laboratory test and dilution, the situation is similar to the one for t = 0 described above. However, in this case the maximum flux is in the opposite direction because $Cs_{eq}$ = 0.

The kinetic sorption model does not differentiate between adsorption and desorption. It is well known that ad- and desorption distribution coefficients may significantly differ. However this fact does not come into conflict with the kinetic sorption model, as long as both, $Kf_{eq}$ and $Kf_{neq}$, refer to either ad- or desorption because the parameter fitted is not $Kf_{neq}$ but the ratio fne. This ratio (fne) is assumed to be equal for ad- and desorption.

The concentrations described in the kinetic sorption model are not measured directly, but should be calculated from the experimental data. The experimental soil system can be considered as given in Figure 4. Each beaker describes the system before removal of the corresponding supernatant.

after application                after centrifugation              after multiple
                                   with $CaCl_2$                    centrifugations
                                                                with organic solvents



$C_w * V_w$

morg S
potentially of
multiple steps

$C_w * V_{p\,0}$

P, $m_0$

$C_{w1} * V_{p\,1}$

P, centr, $m_0$

$m_{org\,P}$

P, centr, $m_0$

**Figure 4: Experimental study design and parameter definitions for each extraction step**

$m_0$      dry soil mass
$V_{p\,0}$     water in pore volume at the beginning ( interstitial water volume)
$V_{p\,1}$     water in pore volume after the first extraction step
$C_w$      concentration in the dissolved phase at the beginning
$C_{w1}$     concentration in the dissolved phase after the first extraction step
$m_{org\,P}$   substance mass in the pore volume filled with organic solvents
$m_{org\,S}$   substance mass in the organic supernatant
P       pore volume

## Appendix 5: Information on Crop Rotations (partly in German)

An overview on the percentage of major field crops as actually found in counties in Germany in 2007 is given in table 5.1.

**Table 5.1: Percentage of major field crops on county level in Germany (in % of arable crop land 2007)**

| Field crop / Percentage of arable land (%) | Winter oilseed rape | Sugar beet | Potatoes | Maize | Winter wheat |
|---|---|---|---|---|---|
| Arithm. average | 10 | 3 | 2 | 15 | 22 |
| 50th percentile | 9 | 1 | 1 | 11 | 23 |
| 90th percentile | 21 | 11 | 6 | 37 | 38 |
| 95th percentile | 23 | 16 | 10 | 45 | 43 |
| 98th percentile | 25 | 22 | 18 | 53 | 47 |
| 99th percentile | 27 | 23 | 20 | 57 | 49 |

Ref: According to Bodennutzungshaupterhebung (BoHa) Kreise 2007.
https://www-genesis.destatis.de/genesis/online/online & Kleffmann GmbH, modified, own calc.
Note: In some communities in Germany the fraction of the crop maize accounts for up to ca. ⅔ of the arable crop land.

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Recommendations for the maximum percentages of individual crops are given in table 5.2 (KTBL 2005, according to Baeumer 1992).

**Table 5.2: Recommended maximum percentage of field crops in a rotation (in % of arable crop land)**

| Field crop | Favorable site | Unfavorable site |
|---|---|---|
| Potatoes | 33 | 25 |
| Sunflower | 17 | 12 |
| Linseed | 14 | 12 |
| Sugar and fodder beets | 33 | 25 |
| Oilseed rape | 33 | 25 |
| Beta beets and all cruciferae | 33 | 25 |
| Field (broad) beans | 25 | 20 |
| Peas | 20 | 17 |
| Leguminosae (seeds) overall | 25 | 20 |
| Wheat | 66 | 50 |
| Winter barley | 40 | 33 |
| Rye, Triticale | 66 | 50 |
| Winter cereals overall | 75 | 67 |
| Spring barley | 50 | 33 |
| Oats | 25 | 25 |
| Spring cereals overall | 50 | 50 |
| Grain cereals overall | 75 | 75 |
| Grain maize | 50 | 33 |
| Maize for silage | 50 | 33 |

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Samples of typical and recommended crop rotations for some field crops in Germany are listed in the following...

## Sugar beets

Sugar beets, winter wheat, winter barley

Sugar beets, winter wheat, winter wheat

Sugar beets, potatoes, winter wheat, winter barley (or winter rye)

## Winter oilseed rape

Winter oilseed rape, winter wheat, winter barley

Winter oilseed rape, winter wheat, winter wheat

Winter oilseed rape, winter wheat, field beans (broad beans), winter barley

Winter oilseed rape, winter wheat, winter wheat, winter barley

Winter oilseed rape, winter wheat, potatoes, winter barley

## Potatoes

Potatoes, maize (for silage), maize (for silage)

Potatoes, winter wheat, winter barley

Potatoes, winter wheat, winter barley, maize (for silage), oats

Potatoes, maize (for silage or grain harvest), rye

Potatoes, maize (for silage or grain harvest), wheat

## Maize (for silage), maize (grain harvest)

Maize (for silage), maize (for silage), potatoes

Maize (grain harvest), maize (grain harvest), winter wheat, winter wheat

Maize (for silage), winter wheat, winter barley (or winter rye), clover-grass mix

Maize (for silage), maize (for silage), winter rye

## Field (broad) beans

Field beans, winter oilseed rape, winter wheat, winter barley

Field beans, winter wheat, winter barley, sugar beets

## Fodder peas

Fodder peas, winter wheat, winter barley

Fodder peas, winter oilseed rape, winter wheat

Fodder peas, winter wheat, winter oilseed rape, winter wheat

Fodder peas, winter wheat, winter barley, winter wheat

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Fodder peas, winter wheat, winter barley, sugar beets

Fodder peas, winter barley, sugar beets, winter wheat


**Cabbage**

Crop rotations with cabbage depend on cabbage species and production type of farming, agricultural or horticultural.


**Cabbage rotations in agriculture**

Winter wheat, carrots, white cabbage, field beans, potatoes

Potatoes, white cabbage, carrots, fodder peas, green manure / inter cropping

Sugar beets, cereals (mainly: winter wheat), head cabbage

Cereals, head cabbage (or curly kale / Grünkohl), cereals


**Cabbage rotations in horticulture**

Vegetables (no brassicas), cabbage, vegetables (no brassicas)

Vegetables (no brassicas), cabbage, cereals

Cabbage, cabbage, vegetables (no brassicas)


Broccoli and / or cauliflower for example may be planted twice a year under favourable growing conditions, after which a period of four years without growing of cabbage species (no brassicas, no cruciferous intercrop) must follow:

Maize, sugar beets, wheat, cauliflower or broccoli (followed by four years without cabbage).

Other cabbage species and other cruciferous are not allowed as intercrop, because this would increase disease pressure (clubroot (Kohlhernie), alternaria (Adernschwärze), seedling diseases such as Phoma (Umfallkrankheit), nematodes, Sclerotinia).

Lettuce and broccoli/cabbage can been grown twice in the same year on the same field. Afterwards lettuce should not be planted again for two years and cabbage should not be planted for four years.

To set up crop rotations for horticultural farms, however, is difficult, because such farms may exchange fields for special crop production with neighbouring farms.


**Lettuce**

Year 1: Lettuce, Chinese cabbage, lettuce [lettuce, lettuce, Chinese cabbage]

Year 2: Winter wheat (planting in autumn of year 1)

Year 3: Sugar beets

Year 4: Lettuce, Chinese cabbage, lettuce

Lettuce as a short cycle crop is often grown twice a year on the same field. Between the two or after the second lettuce crop a further crop, frequently for example Chinese cabbage, is planted.

**Carrots**

Carrots, winter wheat, sugar beets, winter wheat, carrots


**Strawberries**

Strawberries, strawberries (in the field the strawberry crop is grown over two years without replanting), cereals


**Onions**

Onions (dry onions) can be grown again after a minimum non cropping period of three years. Usually the non cropping period is about to be four to six years. This is also valid for Welsh onions and bunching onions.

Crop rotation on loamy soils:

Sugar beet, winter wheat, onions, winter wheat, sugar beet, winter wheat

Onions, winter wheat, sugar beets

Crop rotation on light sandy soils:

Potatoes, winter wheat, onions, winter wheat, potatoes, winter wheat, onions, winter wheat. Winter wheat (in some of the years) can be substituted by winter barley.

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