**Concept for refined FOCUS exposure simulations with PERKLA (CaCN2)**

*Background and motivation*

In order to evaluate the potential risk for surface water organisms after applications of PERKLA on agricultural fields SCHER (2016) has presented standard computer simulations using the FOCUS surface water models and FOCUS scenarios. PERKLA is a formulation (granules) which contains CaCN2 as a fertiliser. It is applied to the field by a tractor mounted with suitable equipment to distribute the formulation equally. Due to the application technique, spray drift should not add to the contamination of surface water. This entry route was therefore not taken into consideration by SCHER (2016). Instead, the CN22- concentrations in surface water were based on drainage and run-off entries. Due to the high dose of 450 kg/ha per year (worst case scenario) especially the concentrations induced by run-off events exceeded the ecotoxicological trigger significantly. An overview about their results is presented in the following table:

**Table: PECsw – FOCUS modelling results for CaCN2 in surface waters according to SCHER (2006)**

|  |  |  |
| --- | --- | --- |
| **Scenario**  | **Maximum PECsw (μg/L) after applying 225 kg/ha** | **Maximum PECsw (μg/L) after applying 450 kg/ha** |
| Drainage D3,ditch | 0.0 | 0.0 |
| Drainage D4,pond | 0.006 | 0.012 |
| Drainage D4,stream | 0.028 | 0.056 |
| Drainage D5,ppond | 0.0 | 0.0 |
| Drainage D5,stream | 0.0 | 0.0 |
| Drainage D6,ditch | 7.5 | 15 |
| Run-off R1,pond | 0.12 | 0.24 |
| Run-off R1,stream | 6.6 | 13 |
| Run-off R2,stream | 220 | 440 |
| Run-off R3,stream | 2300 | 4600 |
| Run-off R4,stream | 3400 | 6800 |

The four run-off scenarios represent situations in Germany (R1, Weiherbach), Portugal (R2, Porto), Italy (R3, Bologna) and southern France (R4, Roujan).

The simulations by SCHER (2016) were based on the assumption that at the time of application the granules instantaneously and completely hydrolyse to hydrogen cyanamide that then directly partitions to soil water. This assumption led to the extremely high concentrations in the surface water body (*e.g.,* 6800 µg/L) at the edge of the agricultural field shortly after the run-off event.

It is the intention of this study to refine the FOCUS simulations by considering additional processes that are relevant for an adequate risk assessment of PERKLA.

*Refinement strategy*

As previously explained the cyanamide concentrations in the different FOCUS surface water scenarios are mainly driven by the high concentrations in soil water directly after application. Though SCHER (2016) considered a short half-life of 2 days for the transformation of cyanamide (at standard laboratory conditions *i.e.,* 20 °C and soil moisture of pF 2), but this degradation rate was finally not substantial due to the short time between PERKLA application and run-off event in the FOCUS scenarios.

It is however reasonable to assume that the granules will not instantaneously hydrolyse to hydrogen cyanamide. Instead, dependent on the climate conditions before the run-off event significant amount of PERKLA may still exist as CaCN2.

As the FOCUS models are able to consider the fate of transformation products the slow release of CaCN2 in granules could be principally considered in the models. The idea is to define a cascade of compounds for the refined FOCUS simulations instead of only cyanamide as done by SCHER (2016):

PERKLA -> hydrogen cyanamide -> urea

However, for the refinement it is essential to determine the hydrolysis of CaCN2 in PERKLA and the formation of urea under different experimental conditions to obtain meaningful input parameters for the FOCUS models.

Following situations with regard to the formation of hydrogen cyan amide should be covered by the experimental studies:

* Application to the soil surface and incorporation into the soil
* Different soil types (considering the properties of the FOCUS scenario soils)
* Different soil temperatures to consider the climatic conditions at the FOCUS locations.
* Different soil moisture

Based on these results more realistic estimation of cyan amide in soil water are expected for the FOCUS simulations before the run-off event. This will lead to simulations that better describe the transport of cyanamide via run-off and should significantly reduce the calculated maximum CN22- concentrations in the surface water bodies at the edge of the agricultural field.

It can be further assumed that the PERKLA granules themselves will not reach surface water directly since this would require agricultural fields with significant slope. However, as PERKLA will not be applied on such fields this direct transport of granules into the surface water bodies can be excluded.