**DRAFT**

**Study Report**

Moisture and Temperature correction of experimentally determined DT50 values for calcium cyanamide and cyanamide according to FOCUS

**Sponsor**

AlzChem Trostberg GmbH

Dr.-Albert-Frank-Str. 32

83308 Trostberg

Germany

**Institute**

Fraunhofer-Institute for Molecular  
 Biology and Applied Ecology (IME)

Auf dem Aberg 1

57392 Schmallenberg  
 Germany

**Director Applied Ecology** Prof. Dr. Christoph Schäfers

**Author**Dr. Michael Klein

Dr. Judith Klein

May 15, 2019

This page was intentionally left blank for statements of the sponsor or submitter.

Statement of compliance

This study “*Moisture and Temperature correction of experimentally determined DT50 values for calcium cyanamide and cyanamide according to FOCUS”*” was conducted according to the procedures described herein. This report is a true and accurate record of the results obtained. There were no circumstances that may have adversely impacted the quality or integrity of the study.

The GLP-regulation is not applicable. However, the study was performed in accordance to the “Codex of Good Modelling Practices” (Görlitz 1993 und Travis 1995).

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_ \_\_15 May\_\_\_\_\_\_

Dr. Michael Klein Date

Exposure Modelling

Fraunhofer Institute

Auf dem Aberg 1

57392 Schmallenberg

Tel +49 2972 302 317

Fax +49 2972 302 319

michael.klein@ime.fraunhofer.de

**Contents page**

[Statement of compliance 3](#_Toc5803152)

[1. Summary 5](#_Toc5803153)

[2. Methodology 6](#_Toc5803154)

[2.1 Moisture correction 6](#_Toc5803155)

[2.2 Temperature correction 7](#_Toc5803156)

[3. Results 8](#_Toc5803157)

[3.1 Calcium cyanamide 8](#_Toc5803158)

[3.2 Cyanamide 11](#_Toc5803159)

[4. References 13](#_Toc5803160)

# Summary

This document explains how experimentally determined DT50 values were corrected according to FOCUS (2000). The models require DT50 values at normalised conditions so that they can be used as input parameters for the calculation of PECsoil, PECsw and PECgw. Laboratory degradation studies are undertaken at various moisture contents often between 40-50% MWHC (**M**aximum **W**ater **H**olding **C**apacity) and at different temperatures (e.g. 10 °C, 12 °C, 20 °C). The actual conditions are influencing the results. Therefore, according to FOCUS (2000) a special procedure called “normalisation” has to be performed before an average value can be calculated.

# Methodology

## Moisture correction

Laboratory degradation studies are undertaken at various moisture contents often between 40-50% MWHC (**M**aximum **W**ater **H**olding **C**apacity). Additional data provided in study reports may include the actual moisture content of the soil during the study expressed volumetrically (% volume/volume), or as gravimetrically (% mass/mass). Other studies may define the reference soil moisture in terms of % field capacity (FC), or as metric potential values such as 10 kPa, 1/3 Bar. The pressure of 10 kPa is often expressed as pF2 which is the decadic logarithm of the same pressure in hekto Pascal. According to FOCUS (2000) a special procedure called “normalisation” has to be performed before an average value can be calculated. **After the normalisation procedure the DT50 at study conditions are transferred to the soil moisture at field capacity (FC). It is assumed that this reference soil moisture content is related to a pressure of 10 kPa (pF2).**

For the normalisation following equation is used:



DT50pf2: DT50 value at moisture content pF2 (normalised condition)

DT50exp: DT50 value at experimental conditions

Θexp: experimental soil moisture

ΘpF2: normalised soil moisture (pF 2)

The equation is identical to the correction of degradation rates that is made in the FOCUS models. The basis for the equation is the assumption that field capacity (pF 2) represents the optimum soil moisture for degradation. If the soil moisture is below field capacity the FOCUS models will unavoidable reduce the degradation rate.

Consequently, the normalisation to field capacity should not be done if faster degradation is observed at lower soil moisture than field capacity. In such a situation the non-normalised values have to be used in risk assessment.

Furthermore, the default soil moisture correction in the FOCUS models should be switched off by setting the soil moisture exponent to “0”.

## Temperature correction

Laboratory degradation studies are undertaken at various temperatures 10 °C and 25 °. However, the FOCUS models require the degradation rates (or half lives) at 20 °C (normalised conditions). Therefore, according to FOCUS (2000) a special procedure called “normalisation” has to be performed before an average value can be calculated.

For the normalisation following equation is used:



DT5020°C: DT50 value at 20 °C (normalised condition)

DT50exp: DT50 value at experimental conditions

Texp: Temperature during study (in °C)

# Results

## Calcium cyanamide

In the following table the resulting normalised DT50 values are presented for the transformation of calciumcyanamide to cyanamide before and after normalising the DT50 values to a temperature of 20°C:

**Table 1: Temperature normalisation of DT50 values of calcium cyanamide to reference conditions (20 °C)**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Name** | **Reference** | **Soil type** | **DT50 at study conditions**  **(days)** | **Temperature**  **(°C)** | **Normalisation factor** | **DT50 after normalisation**  **to 20 °C (days)** |
| Refesol 01-A | Güthner (2018) | Loamy sand | 1.1 | 12 | 0.532 | 0.585 |
| Refesol 01-A | Güthner (2018) | Loamy sand | 1.8 | 12 | 0.532 | 0.958 |
| Refesol 01-A | Weinfurtner (2019) | Loamy sand | 0.6 | 20 | 1.000 | 0.600 |
| Refesol 01-A | Weinfurtner (2019) | Loamy sand | 1.21 | 20 | 1.000 | 1.210 |
| Refesol 02-A | Weinfurtner (2019) | Silt loam | 0.87 | 12 | 0.532 | 0.463 |
| Refesol 02-A | Weinfurtner (2019) | Silt loam | 1.63 | 12 | 0.532 | 0.867 |
| Refesol 06-A | Weinfurtner (2019) | silty clay | 2.51 | 20 | 1.000 | 2.510 |
| Refesol 06-A | Weinfurtner (2019) | silty clay | 2.47 | 20 | 1.000 | 2.470 |
| Dugliolo di Budrio | Weinfurtner (2019) | Silt loam | 1.61 | 20 | 1.000 | 1.610 |
| Dugliolo di Budrio | Weinfurtner (2019) | Silt loam | 1.63 | 20 | 1.000 | 1.630 |
| **Geometric mean** | |  | **1.42** |  |  | **1.10** |

After normalisation to 20 °C the geometric mean of all DT50 values changed from 1.42 d to 1.10 d.

In the following table the DT50 values at 20 °C from the table above were used for the additional soil moisture normalisation.

**Table 2: Soil moisture normalisation of DT50 values (20 °C) of Calcium cyanamide to reference conditions (pF 2)**

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Name** | **Reference** | **Soil type** | **DT50 at  20 °C (days)** | **exp. soil moisture (%)** | **reference soil moisture (%)** | **normalisation factor** | **DT50 after normalisation to 20 °C and FC (days)^** |
| Refesol 01-A | Güthner (2018) | Loamy sand | 0.585 | 10 | 12 | 0.880 | 0.515 |
| Refesol 01-A | Güthner (2018) | Loamy sand | 0.958 | 5 | 12 | 0.542 | 0.519 |
| Refesol 01-A | Weinfurtner (2019) | Loamy sand | 0.600 | 10 | 12 | 0.880 | 0.528 |
| Refesol 01-A | Weinfurtner (2019) | Loamy sand | 1.210 | 5 | 12 | 0.542 | 0.656 |
| Refesol 02-A | Weinfurtner (2019) | Silt loam | 0.463 | 21 | 26 | 0.861 | 0.399 |
| Refesol 02-A | Weinfurtner (2019) | Silt loam | 0.867 | 10.4 | 26 | 0.527 | 0.457 |
| Refesol 06-A | Weinfurtner (2019) | silty clay | 2.510 | 16 | 46 | 0.477 | 1.198 |
| Refesol 06-A | Weinfurtner (2019) | silty clay | 2.470 | 32 | 46 | 0.776 | 1.916 |
| Dugliolo di Budrio | Weinfurtner (2019) | Silt loam | 1.610 | 9.1 | 26 | 0.480 | 0.772 |
| Dugliolo di Budrio | Weinfurtner (2019) | Silt loam | 1.630 | 18.2 | 26 | 0.779 | 1.270 |
| **Geometric mean** | |  | **1.10** |  |  |  | **0.721** |

\* These are default values taken from FOCUS (2000)   
^ The optimised soil moisture is field capacity (FC) according to FOCUS (2000)

For FOCUS surface and groundwater modelling a DT50 of 0.72 days should be used. The value represents the geometric mean of all experimental results after normalisation to 20 °C including soil moisture normalisation.

For modelling PEC soil with ESCAPE [Klein 2008] the DT50 of 1.10 should be used, because ESCAPE does not calculate the degradation dependent on soil moisture conditions.

## Cyanamide

For cyanamide no soil moisture normalisation was done since according to the experimental results the degradation of cyanamide does not always increase with soil moisture (see the following table). Consequently, the soil moisture correction in the groundwater model PEARL (FOCUS 2000) and the surface water models MACRO and PRZM (FOCUS 2001) are not suitable and the moisture correction was switched off in the simulation. The geometric mean of the DT50 of all studies without considering temperature normalisation was found to be 0.95 d. However, for the modelling with PEARL, MACRO, and PRZM a DT50 of 0.78 d should be used. This DT50 value represents the geometric mean of all experimental data after normalisation to 20 °C but without soil moisture normalisation. This value is more suitable than the DT50 of 0.95 d because the models require half-lives at 20 °C for their automatic correction to actual scenario conditions. The details of the normalisation can be found in the following table.

**Table 3: Temperature normalisation of DT50 values of cyanamide to reference conditions (20 °C)**

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Name** | **Reference** | **Soil type** | **exp. Temperature (°C)** | **exp. soil moisture\*** | **DT50 at study conditions**  **(days)** | **Normali-sation factor** | **DT50 after normalisation**  **to 20 °C (days)** |
| Refesol 01-A | Güthner (2018) | Loamy sand | 12 | 10% | 2.2 | 0.532 | 1.17 |
| Refesol 01-A | Güthner (2018) | Loamy sand | 12 | 5% | 1.3 | 0.532 | 0.69 |
| Refesol 01-A | Weinfurtner (2019) | Loamy sand | 20 | 10% | 0.95 | 1.000 | 0.95 |
| Refesol 01-A | Weinfurtner (2019) | Loamy sand | 20 | 5% | 0.82 | 1.000 | 0.82 |
| Refesol 02-A | Weinfurtner (2019) | Silt loam | 12 | 21% | 1.15 | 0.532 | 0.61 |
| Refesol 02-A | Weinfurtner (2019) | Silt loam | 12 | 10.4% | 1.06 | 0.532 | 0.56 |
| Refesol 06-A | Weinfurtner (2019) | silty clay | 20 | 16% | 0.42 | 1.000 | 0.42 |
| Refesol 06-A | Weinfurtner (2019) | silty clay | 20 | 32% | 0.55 | 1.000 | 0.55 |
| Dugliolo di Budrio | Weinfurtner (2019) | Silt loam | 20 | 9.1% | 1.21 | 1.000 | 1.21 |
| Dugliolo di Budrio | Weinfurtner (2019) | Silt loam | 20 | 18% | 0.79 | 1.000 | 0.79 |
| Ashland | EFSA (2010) | Sandy Loam | 20 | - | 0.70 | 1.000 | 0.70 |
| SP 257 | EFSA (2010) | Loamy sand | 20 | - | 0.96 | 1.000 | 0.96 |
| SP 357 | EFSA (2010) | Loamy sand | 20 | - | 1.24 | 1.000 | 1.24 |
| **Geometric mean** | |  |  |  | **0.95** |  | **0.78** |

\* this information was not considered for the normalisation

# References

EFSA (2010): Conclusion on the peer review of the pesticide risk assessment of the active substance cyanamide. EFSA Journal 2010;8(11):1873. page 30 doi:10.2903/j.efsa.2010.1873. Available online: www.efsa.europa.eu/efsajournal.htm

FOCUS (2000): “FOCUS groundwater scenarios in the EU review of active substances”. Report of the FOCUS Groundwater Scenarios Workgroup, EC Doc. Ref. SANCO/321/2000 rev. 2; and “Generic guidance for FOCUS groundwater scenarios”. FOCUS Groundwater Scenario Workgroup, May 2001, Version

FOCUS (2001). “FOCUS Surface Water Scenarios in the EU Evaluation Process under 91/414/EEC”. Report of the FOCUS Working Group on Surface Water Scenarios, EC

FOCUS (2007). “Landscape And Mitigation Factors In Aquatic Risk Assessment. Volume 1. Extended Summary and Recommendations”. Report of the FOCUS Working Group on Landscape and MitigationFactors in Ecological Risk Assessment, EC Document Reference SANCO/10422/2005 v2.0. 169 pp.

Görlitz. G. (1993): Verfahrensregeln zur korrekten Durchführung und Auswertung von Modellrechnungen zur Simulation des Umweltverhaltens von Pflanzenschutzmitteln.

Güthner T. (2018), Transformation of Perlka in Soil: Determination of Free Cyanamide and Modelling of Degradation Kinetics, Trostberg 28.12.2018

Klein (2008): Calculation of PECsoil including Plateau Concentrations for Pesticides Dependent on FOCUS Degradation Kinetics. User Manual ESCAPE Version 2. Fraunhofer-IME. Schmallenberg.

Travis. K.Z. (1995): Recommendations for the correct use of models and reporting of modelling results.- in: ‘Leaching Models and EU registration’. Final report of the FOCUS Group. Doc. 4952/VI/95.

Weinfurtner, K. (2019): Release and Transformation of Cyanamide from PERLKA®, Fraunhofer Institute for Molecular Biology and Applied Ecology (IME), Schmallenberg, April.2019