Fraunhofer IME

Study Report

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

Sponsor

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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).

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1. 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.

2. Methodology

2.1 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:

$$DT50_{pF2} = DT50_{exp} \cdot \left(\frac{\Theta_{exp}}{\Theta_{pF2}} \right)^{0.7}$$

$DT50_{pf2}$:	DT50 value at moisture content pF2 (normalised condition)
$DT50_{exp}$:	DT50 value at experimental conditions
Θ_{exp}:	experimental soil moisture
Θ_{pF2}:	normalised soil moisture (pF 2)

2.2 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:

$$DT50_{20\,°C} = DT50_{exp} \cdot 2.2^{\frac{T_{exp}-20}{10}}$$

$DT50_{20°C}$: DT50 value at 20 °C (normalised condition)

$DT50_{exp}$: DT50 value at experimental conditions

T_{exp}: Temperature during study (in °C)

3. Results

3.1 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.

3.2 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

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