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# An improved soil organic matter map for GeoPEARL\_NL

Model description of version 4.4.4 and consequences for the Dutch decision tree on leaching to groundwater

F. van den Berg, A. Tiktak, T. Hoogland, A. Poot, J.J.T.I. Boesten, A.M.A. van der Linden, J.W. Pol



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# An improved soil organic matter map for GeoPEARL\_NL

Model description of version 4.4.4 and consequences for the Dutch decision tree on leaching to groundwater

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GeoPEARL\_NL is used as a higher tier instrument in the leaching assessment of plant protection products in the Netherlands. Because the soil organic matter contents in arable soils in the current version were too high, a new soil organic matter for the Netherlands was needed. The new 3D organic matter map has been generated in two steps; first a trend model was developed based on data at 1210 locations selected using a well-defined stratified random sampling scheme followed by interpolation of the residuals using about 770 000 determinations of organic matter content from the Dutch Soil Information System (BIS-Nederland). In general, the predicted soil organic matter contents in the top layer of arable soils correspond well with those measured. Because preliminary calculations showed higher leaching concentrations using the new GeoPEARL version, the consequences of this new version in combination with the Dutch Decision Tree for leaching to groundwater was investigated. The results of the computations revealed that the PEC90 calculated using GeoPEARL in tier 2 is higher than the PEC80 calculated using FOCUSPEARL in many cases. This inconsistency between the first and second tiers could be remedied by the introduction of a calibration factor. Calibration factors of 5 and 10 are necessary to ensure consistency between these tiers for spring and autumn applications, respectively. Suggestions are given for improvement and justification of the calibration factors in the Decision Tree. It is recommended to systematically compare the predicted leaching concentration in groundwater abstraction areas with that in the Dutch agricultural area as a whole. To improve the reliability of model predictions for these smaller areas, development a more flexible schematisation is needed.

Keywords: decision tree, GeoPEARL, groundwater, leaching, national authorisation, plant protection product, pesticide, soil organic matter

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# Preface

During the development of the improved methodology for the assessment of effects on aquatic organisms, the Dutch Working Group on Exposure of Aquatic Organisms discovered an error in the organic matter content in the top soil of arable soils as used in the soil schematisation of GeoPEARL. Analysis of the data showed that the organic matter content in the top 0.3 m of arable soil profiles in GeoPEARL was 1.5 to 2 times higher than that measured in these soils. This difference was introduced in the schematisation at the time of the development of the schematisation, because the aim was to estimate the average organic matter content in a grid cell, which results from a mixture of grassland and arable soil profiles. The consequence of the error in the organic matter content of arable soils is that the leaching concentrations to groundwater are underestimated. To remedy this, the Working Group on the Dutch Decision Tree for Leaching to Groundwater started to work on the improvement of the soil schematisation for GeoPEARL in 2013. The Working Group also had to check whether the GeoPEARL version based on this improved schematisation was still consistent with the Decision Tree and was to propose new calibration factors if necessary.

The development of the improved soil organic matter map and its implementation in the schematisation of GeoPEARL is described in this report. The consequences of the new version and its use in the Decision Tree for leaching are discussed and new calibration factors are proposed for tier 1 calculations with the Kremsmünster scenario using FOCUSPEARL in order to make it consistent with tier 2 calculations using GeoPEARL. In addition, recommendations are made for further analysis of the calibration factor for 1) substances with properties not included in the testing done so far and 2) the groundwater protection areas.





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# Summary

GeoPEARL is used as a higher tier instrument in the leaching assessment of plant protection products in the Netherlands. In 2010, it was noted that the soil organic matter contents in arable soils as included in the current schematisation of GeoPEARL (v 3.3.3) were too high compared with measured values in these soils. The soil organic matter map of the versions that have been released so far was based on soil profile information from all agricultural soils, so data from arable as well as from grassland fields were used. However, the organic matter content in the top layer of arable soils is substantially lower than in the top layer of grassland soils. As soil organic matter content is one of the key factors influencing leaching of plant protection products to groundwater it was evident that a new soil organic matter map was needed.

A methodology was developed to predict the organic matter content in soils at different depths. The new 3D organic matter map has been generated using a two-step procedure. Firstly, a trend model was developed based on data from the Soil Sampling Program for the Netherlands and mapped soil type and land-use (arable or grassland) as predictors. This dataset contains recent measurements of soil organic matter at 1210 locations selected using a well-defined stratified random sampling scheme. The second step consisted of an interpolation of the residuals of the trend model based on about 770 thousand measurements of organic matter content from the Dutch Soil Information System (BIS-Nederland). In this way, regional differences in organic matter content within soil map units are taken into account.

The resulting 3D soil organic matter map has a resolution of 250 x 250 m in the horizontal plane and predicts the organic matter content at fixed depths of 15, 45, 80 and 120 cm below the soil surface. Because the organic matter content in the top layer in arable soils is lower than that in grassland soil, separate procedures were developed for the prediction of organic matter contents in the top layer of arable and grassland fields. For subsoil layers there is no effect of land use in the model to predict the soil organic matter content. The predicted soil organic matter contents in the top layer of arable fields were compared with measurements of the organic matter content in top soil samples taken to assess the fertility of the soil (the Reijneveld dataset). In general, there is a good agreement between the predicted contents in the new map and the measurements in soils, except for peaty soils. This difference can be partly explained by the fact that the Reijneveld samples were collected in the period 1994-2001, so the decrease in the organic matter content due to oxidation since then is not accounted for in the comparison.

The soil schematisation of GeoPEARL version 3.3.3 contains descriptions of the organic matter content in 456 soil profiles. In order to correct the organic matter contents in these soil profiles, the median organic matter content was calculated for each depth considering only the grid cells that are linked with a specific soil profile. This aggregation to soil profile areas resulted in heterogeneity in soil organic matter content within these soil profile areas. Therefore, an aggregation to STONE plots was also investigated. This aggregation resulted in much less heterogeneity in organic matter content within plots, so this aggregation was adopted for the new GeoPEARL schematisation.

Preliminary calculations were done for 120 substances covering a wide range of values of DegT50 (range 20 to 200 d) and  $K_{om}$  (range 0 to 250 L kg<sup>-1</sup>) with a yearly application on 26 May in maize, cereals and flower bulbs. The results showed that leaching concentrations increase by a factor 2 to 3 for the spring application in cereals and flower bulbs and up to a factor 10 for the spring application in maize. Therefore, the consequences of the new version of GeoPEARL in combination with the Dutch Decision Tree for leaching to groundwater was investigated to find out what modifications are needed to ensure consistency between the first and second tiers of this assessment scheme.

In the first tier, the Kremsmünster scenario is used and the 80 percentile of the leaching concentrations is calculated by FOCUSPEARL. In tier 2 of the Decision Tree the 90<sup>th</sup> percentile leaching

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concentration in space is calculated by GeoPEARL in the area of use of the compound. A set of 20 substances was selected which covered the range of interest of  $K_{om}$  and DegT50 combinations. The value of the Freundlich exponent was set to 0.9 in all cases. The application dates considered in the computations were the 15<sup>th</sup> of each month. Computations were done for all crop - substance - application date combinations using the tier 1 FOCUS Kremsmünster scenario with FOCUSPEARL and the corresponding tier 2 scenarios with the new GeoPEARL schematisation.

The results of the computations revealed that the PEC90 calculated using GeoPEARL in tier 2 is higher than the PEC80 calculated using FOCUSPEARL in many cases. To remedy this inconsistency between the first and second tiers a calibration factor was introduced, which is defined as the factor with which the FOCUS leaching concentration from the Kremsmünster scenario has to be multiplied to ensure that the endpoint of tier 1 is more conservative than the corresponding calculation in tier 2 using GeoPEARL. For spring applications, i.e. in the period from 1 March to 31 August, a calibration factor of 5 is necessary to ensure consistency between these tiers. For autumn applications, i.e. in the period from 1 September to 29 February, a calibration factor of 10 is necessary to maintain a consistent decision tree for most substances.

On the basis of the findings in this report, it is no longer necessary to make an exception for flower bulbs as described in the Dutch evaluation manual of Ctgb, neither is it necessary to skip tier 1 for compounds with a  $K_{om}$  of less than 10 L kg<sup>-1</sup> and a DegT50 of less than 10 d as specified in the 2004 Decision Tree. There could be an additional criterion to ensure consistency for all crop - substance combinations for applications in the period of September to February. For most substances in the non-consistent cases the ratio of  $K_{om}$  to DegT50 is about 4. So full consistency could be maintained by introducing a criterion that for compounds with a ratio of  $K_{om}$  to DegT50 in the range of 3.5 to 4.5 tier 1 calculations could be skipped, so for these compounds Tier 2 assessments always need to be done.

The proposed calibration factors are based on calculations using a Freundlich exponent of 0.9. Checks for two substances showed that these calibration factors may not be conservative enough for a Freundlich exponent of 0.8, which is usually the lowest average value found in dossiers. To make the tiered approach consistent for all possible substances, it is recommended to estimate also the calibration factors for compounds with a Freundlich exponent of 0.8. Consistency of the tiered approach has further not been checked for relevant soil metabolites, so further checks on leaching concentrations of metabolites are recommended.

Depending on the crop, the organic matter content in groundwater abstraction areas can be either lower or higher than in the Dutch agricultural area as a whole. This implies that the 90<sup>th</sup>-percentile of the leaching concentration in groundwater abstraction areas can be either higher or lower than the concentration in the Dutch agricultural area as a whole. Therefore it is not evident that a factor of 10 that is currently used to protect groundwater abstraction areas is always necessary. We therefore recommend to systematically compare the predicted leaching concentration in groundwater abstraction areas with that in the Dutch agricultural area as a whole.

The current schematisation of GeoPEARL consists of 6 405 fixed unique combinations of soil type, drainage system, climate district and land-use type (so-called plots). This leads to uncertainty of the model predictions for smaller areas, e.g. for individual groundwater abstraction areas and for less common crops like asparagus and onions. To improve the reliability of model predictions for these smaller areas, a more flexible schematisation procedure that allows for the derivation of unique combinations that overlap entirely with the areas of interest would be needed. This is not possible with the current STONE schematisation. We therefore recommend to link with current efforts to develop a revised STONE schematisation using NHI, the Netherlands Hydrological Instrument, which is the new consensus model for Dutch water management. Because this instrument is intended to perform calculations at a high spatial resolution (grid cell size of 250 by 250 m), dedicated unique combinations of grid cells can be derived for any given target area, e.g. one of the groundwater abstraction areas.

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# Samenvatting

GeoPEARL wordt gebruikt in een hogere stap van de uitspoelingsbeoordeling van gewasbeschermingsmiddelen in Nederland. In 2010 werd geconstateerd dat het gehalte aan organische stof in akkerbouwgronden in de huidige schematisatie van GeoPEARL (v. 3.3.3) te hoog was in vergelijking met de gemeten gehalten in deze gronden. De organische-stofkaart die GeoPEARL gebruikt was gebaseerd op gehalten in alle gronden in het landbouwkundig areaal, waarbij geen onderscheid werd gemaakt tussen akkerland en grasland. Het organische-stofgehalte in de toplaag van akkerland gronden is echter substantieel lager dan in de toplaag van grasland gronden. Aangezien het organische-stofgehalte een van de bepalende factoren is die invloed heeft op de uitspoeling van deze middelen naar het grondwater was duidelijk dat een vernieuwde organische-stofkaart nodig was.

Een methodiek werd ontwikkeld om het organische stofgehalte te voorspellen op verschillende dieptes. De nieuwe 3-D organische stofkaart werd gemaakt in 2 stappen. Eerst werd een trendmodel ontwikkeld met behulp van gegevens van de Landelijke Steekproef Kaarteenheden met het bodemtype op de bodemkaart van Nederland en het landgebruik (akkerbouw of grasland) als voorspellende variabelen. De dataset bevat recente metingen van het organische stofgehalte op 1210 locaties die geselecteerd werden via een gestratificeerde selectie methode. De tweede stap bestond uit een interpolatie van residuen van het trendmodel op basis van 770 000 metingen van organische stof afkomstig van het Bodemkundig Informatie Systeem voor Nederland (BIS-Nederland). Op deze wijze werd rekening gehouden met regionale verschillen in organische stofgehalte.

De gerealiseerde 3D organische-stofkaart heeft een resolutie van 250 bij 250 m en voorspelt het organische stofgehalte op 4 vaste diepten, nl. op 15, 45, 80 en 120 cm. Aangezien het organische-stofgehalte in de toplaag van akkerbouwgronden lager is dan die in graslandgronden werd een aparte procedure gemaakt voor de voorspelling van het gehalte in de toplaag van deze gronden. Voor de ondergrond is er geen effect van landgebruik op de voorspelling. De voorspelde organische-stofgehalten in de toplaag van akkerbouwgronden werden vergeleken met metingen in grondmonsters genomen voor de bepaling van de bodemvruchtbaarheid ('Reijneveld' dataset). Over het algemeen is de overeenkomst goed, behalve voor veengronden. Dat verschil kan deels verklaard worden door het feit dat de monsters van Reijneveld werden genomen in de periode 1994-2001, waardoor geen rekening werd gehouden met een verlaging in het organische-stof gehalte ten gevolge van oxidatie in de jaren erna.

De bodemschematisatie van GeoPEARL versie 3.3.3 bevat een beschrijving van het organische-stofgehalte in 456 bodemprofielen. Om het organische stofgehalte in deze bodemprofielen profielen te corrigeren werd het mediane organische stofgehalte voor elke diepte berekend voor de gridcellen die aan een specifiek bodemprofiel waren gekoppeld. Deze aggregatie tot bodemprofielgebieden resulteerde in heterogeniteit in het organische stofgehalte binnen het gebied van het bodemprofiel. Vervolgens werd een aggregatie naar STONE plots onderzocht. Deze aggregatie resulteerde in veel minder heterogeniteit in het organische stofgehalte binnen de STONE plots; daarom werd deze aggregatie gekozen voor de nieuwe GeoPEARL schematisatie.

Eerst werden berekeningen uitgevoerd voor 120 stoffen met een groot bereik van waarden voor de DegT50 (range van 20 tot 200 d) en de  $K_{om}$  (range van 0 tot 250 L kg<sup>-1</sup>) met een jaarlijkse toediening op 26 mei in mais, granen en bloembollen. Toepassing van de nieuwe GeoPEARL versie resulteerde in uitspoelconcentraties die een factor 2-3 hoger waren voor de voorjaarstoepassing in granen en bloembollen en tot een factor 10 voor de voorjaarstoepassing in mais. Het was dus nodig om de consequenties van het gebruik van de nieuwe GeoPEARL versie in kaart te brengen en na te gaan welke aanpassingen nodig waren in het beoordelingsschema.

In de eerste stap ("tier 1") wordt het Kremsmünster scenario gebruikt om de 80 percentiel uitspoelconcentratie te berekenen met behulp van FOCUSPEARL. In tier 2 wordt de 90 percentiel

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concentratie in de ruimte berekend met GeoPEARL voor het gewasareaal waarin de stof gebruikt wordt. Een set van 20 stoffen werd geselecteerd met eigenschappen die de relevante range van combinaties van waarden voor  $K_{om}$  en DegT50 bestreken. De waarde van de Freundlich exponent werd gezet op 0.9 voor alle stoffen. De gekozen toedieningsdata in de berekeningen waren de 15<sup>e</sup> van elke maand. Berekeningen werden uitgevoerd voor alle gewas – stof – toedieningsdatum combinaties voor het tier 1 Kremsmünster scenario met FOCUSPEARL en met de nieuwe GeoPEARL versie voor de overeenkomstige scenario's in tier 2.

De PEC90 berekend met GeoPEARL in tier 2 was in veel gevallen hoger dan de PEC80 berekend in tier 1 met FOCUSPEARL. Om deze inconsistentie tussen tier 1 en tier 2 te verhelpen, werd een kalibratie factor geïntroduceerd, die gedefinieerd is als de factor waarmee de FOCUS uitspoelconcentratie voor het Kremsmünster scenario moet worden vermenigvuldigd om er voor te zorgen dat het eindpunt van tier 1 conservatiever is dan die van tier 2 met GeoPEARL. Voor voorjaarstoepassingen, d.w.z. in de periode van 1 maart tot en met 31 augustus, is een kalibratiefactor van 5 nodig om consistentie te bewerkstelligen. Voor najaarstoepassingen, d.w.z. van 1 september tot en met 29 februari, is voor de meeste stoffen een kalibratiefactor van 10 nodig om te zorgen voor een consistente beslisboom.

Op basis van de resultaten in dit rapport is het niet langer nodig om een uitzondering te maken voor bloembollen zoals dat aangegeven is in de Nederlandse Evaluatie Handleiding van het Ctgb. Evenmin is het nodig om tier 1 over te slaan voor stoffen met een  $K_{om}$  van minder dan 10 L kg<sup>-1</sup> en een DegT50 waarde van minder dan 10 d, zoals opgenomen in de Beslisboom van 2004. Er zou mogelijk een additioneel criterium opgenomen kunnen worden om de consistentie te garanderen voor alle gewas – stof combinaties in de periode van september tot en met februari. Voor de meeste stoffen in de gevallen waarin er geen consistentie is, is de ratio van  $K_{om}$  en DegT50 ongeveer 4. Dus volledige consistentie zou gehandhaafd kunnen worden door de introductie van het criterium dat voor stoffen met een ratio van  $K_{om}$  en DegT50 tussen 3.5 en 4.5 tier 1 wordt overgeslagen en dat voor dergelijke stoffen altijd berekeningen voor tier 2 dienen te worden uitgevoerd.

De voorgestelde kalibratiefactoren zijn gebaseerd op berekeningen voor stoffen met een Freundlich exponent van 0.9. Controles voor 2 stoffen wezen uit dat de voorgestelde kalibratiefactoren mogelijk niet conservatief genoeg zijn voor stoffen met een exponent van 0.8, wat meestal de laagst gemiddelde waarde is in de stofdossiers. Om het beoordelingsschema consistent te maken voor alle stoffen wordt aanbevolen om ook kalibratiefactoren te schatten voor stoffen met een exponent van 0.8. De consistentie van de beslisboom is ook niet getest voor relevante metaboliëten, dus wordt aanbevolen om dat ook voor metaboliëten te doen.

Afhankelijk van het gewas kan het organische-stofgehalte in grondwateronttrekkingsgebieden lager dan wel hoger zijn dan dat in het totale landbouwkundige areaal. Dat houdt in dat het 90 percentiel van de uitspoelconcentratie in die gebieden ook lager dan wel hoger kan zijn dan in het totale areaal. Het is daarom niet zonder meer duidelijk of de factor 10 die in de huidige beslisboom gebruikt wordt ter bescherming van deze gebieden nodig is. Wij bevelen daarom aan om de voorspelde uitspoelconcentratie in grondwateronttrekkingsgebieden op systematische wijze te vergelijken met die in het totale landbouwkundige areaal.

De huidige schematisatie van GeoPEARL bevat 6450 unieke combinaties van gewastype, drainagesysteem, klimaatdistrict en landgebruik (zgn. plots). Dat leidt tot onzekerheid in de modelvoorspellingen voor kleinere arealen, zoals voor individuele grondwateronttrekkingsgebieden en minder voorkomende gewassen als asperge en uien. Om de betrouwbaarheid van de voorspellingen te vergroten is een meer flexibele schematisatie nodig zodat unieke combinaties afgeleid kunnen worden die het doelgebied volledig bedekken. Aanbevolen wordt om aan te sluiten bij het huidige werk aan de herziening van de STONE schematisatie met behulp van het NHI, dat het nieuwe consensus instrument is voor het Nederlandse Waterbeheer. Aangezien dat instrument berekeningen kan doen met een hoge ruimtelijke resolutie (gridcelgrootte van 250 bij 250 m) kan dan een specifieke set met unieke combinaties van gridcellen verkregen worden voor elk gebied (bijv. één van de grondwateronttrekkingsgebieden).

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# 1 Introduction

GeoPEARL is used as a higher tier instrument in the leaching assessment of plant protection products in the Netherlands (van der Linden et al. 2004). The calculation of leaching is spatially distributed over up to 6405 scenarios which differ from each other in, amongst other, climatic conditions and soil characteristics (Tiktak et al. 2003). The currently used version of GeoPEARL is version 3.3.3, but the underlying geographical information has not been updated since version 1.

The soil organic matter content is one of the key factors influencing leaching of plant protection products to groundwater (van den Berg et al., 2012). In 2010, it was noted that the soil organic matter map in the database of GeoPEARL contained higher values for the organic matter content in the top layer of arable soils in the Netherlands than those measured in top soils reported by Reijneveld et al. (2009). When using too high values, the leaching to groundwater will be underestimated.

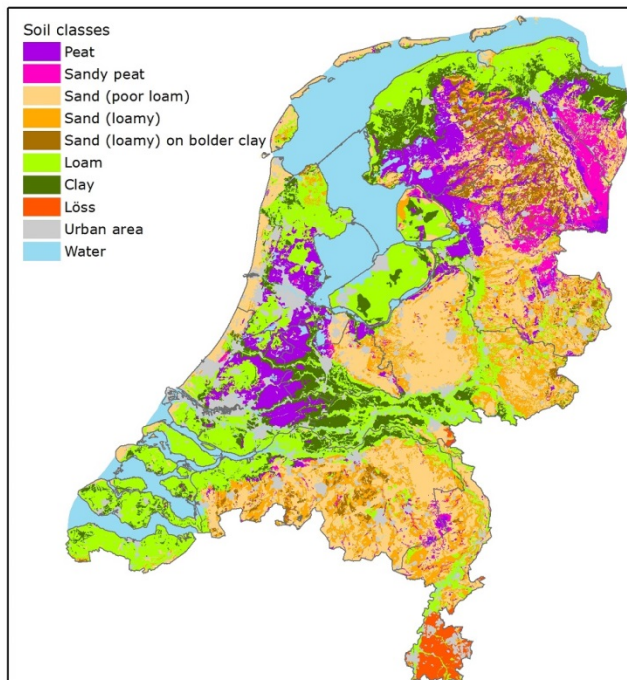
The organic matter map of GeoPEARL version 1.1.1 was generated using profile information from all agricultural soils, i.e. soils from both arable and grassland fields, which in some areas may lead to overestimation of the organic matter content. It was decided to generate new soil organic matter maps, for arable and grassland fields separately.

The new soil organic matter maps became available in 2015 and they were adapted to the GeoPEARL soil and plot schematisation (see Chapter 2) and implemented in the GeoPEARL database. The new GeoPEARL version was used to calculate leaching concentrations for a number of hypothetical substances for all plots of the GeoPEARL schematisation (see Chapter 3). Chapter 3 also describes the comparison of the new and the old version, using different aggregation procedures and for selected crops available in GeoPEARL. Chapter 4 describes the comparison of results of the new GeoPEARL version with results of calculations for the FOCUS Kremsmünster scenario. Consequences for the decision tree on leaching are discussed in Chapters 5 and 6, including suggestions for calibration factors to be used in tier 1 of the decision tree, for both the total crop area in the Netherlands and the crop area in groundwater protection areas. Finally, Chapter 7 gives the overall conclusions and recommendations for further research.

## 2 Materials and methods

The current version of the soil organic matter map in GeoPEARL is based on 456 typical soil profiles which are assigned to soil map units at the 1:50,000 soil map of the Netherlands (De Vries, 1994). The main soil types are shown in Figure 2.1. The consequence is that only one typical value for each soil map unit has been used. Van den Berg et al. (2012) stated that the reliability and precision of the map depicting soil organic matter could be improved by using more measurements of soil organic matter (SOM), or exploiting full coverage information of covariates such as soil type and land-use. This can be achieved by combining maps of soil type with soil property information from thousands of observations on soil organic matter content available in the Dutch Soil Information System (Heuvelink and Bierkens, 1992; Brus et al., 1996). To provide spatially exhaustive and accurate information on SOM contents a trend model is calibrated using the mapped soil type and land-use as a predictor, in combination with interpolation of the residuals (Knotters et al., 1995; Hengl et al., 2004). The new 3D soil organic matter map in GeoPEARL was generated using this method.

The new soil organic matter map is available at a resolution of 250 x 250 m and for four depths (15, 45, 80 and 120 cm). This map can, however, not be used directly in GeoPEARL because the spatial schematization of GeoPEARL is based on 6405 unique combinations (or so-called plots) of hydrological properties, climatic properties, and soil properties. So some sort of aggregation is needed. Aggregation is possible to the level of the 456 soil profiles in GeoPEARL. This is in line with the current schematization of the model, which uses only one value per soil profile. However, the availability of the high-resolution soil organic matter content map makes it also possible to aggregate to the level of the 6405 plots, improving the spatial resolution of the aggregated organic matter map in GeoPEARL by a factor of 14. Both aggregation levels were tested and the consequences reported.



**Figure 2.1** Soil types in the Netherlands (based on Soil map of the Netherlands 1:50000).

The following paragraphs first describe the generation of the full-resolution soil organic matter content map based on geostatistical procedures. Then the procedures for aggregation to the level of GeoPEARL plots are described.

## 2.1 Statistical model of soil organic matter in the Netherlands

The aim of the developed statistical model is to generate exhaustive information on soil organic matter content with a resolution of 250 x 250 meter in the horizontal plane and at fixed depths of 15, 45, 80 and 120 cm below the local soil surface, matching the depth of the GeoPEARL model. To enable risk assessments studies, the accuracy of the predictions is quantified at the same spatial resolution. Soil profile observations and exhaustive covariates derived from the nation-wide soil map are used in a 3D geostatistical interpolation procedure. Here, we present the methodology for an exhaustive 3D-model of soil organic matter content.

### 2.1.1 Soil profile data

The Dutch Soil Information System (BIS-Nederland, Version 7, Wageningen Environmental Research (Alterra)) contains information on soil organic matter content at more than 300 000 locations and for more than 1 million soil layers. The location, depth and year of the soil profile observations were always recorded; the oldest observations are from 1953. Observed soil organic matter content in mineral soils show no clear indication of loss or increase over time, which is in line with Reijneveld et al. (2009) who reported only a very small (non-significant) decrease over time. Because the aim is to predict the present soil organic matter content only soil profiles from 1990 onwards were used up to 2013.

#### *Combining field estimates and laboratory measurements*

The soil information system contains both field estimates of soil organic matter and laboratory measurements. Field estimates are most abundant (total of 780 000 field estimates). For some 20 000 soil horizons laboratory measurements of soil organic matter using loss on ignition at 600 °C were available of which ten thousand have both a laboratory measurement and a field estimate of soil organic matter content. This subset was used to calibrate the field estimates against laboratory measurements according to equation 1:

$$\ln(y_m + 1) = \alpha_0 + \alpha_1 \ln(y_f + 1) + \varepsilon_f \quad (1)$$

where  $\ln(y_m)$  is the log-transformed laboratory measurement of organic matter (%),  $\ln(y_f)$  is the log-transformed field estimate of soil organic matter (%),  $\alpha_0$  and  $\alpha_1$  are regression coefficients and  $\varepsilon_f$  is the estimation error. The values of the regression coefficients given in Table 2.1 indicate a significant difference between field estimates for organic matter content and laboratory measurements, showing the need for this correction. This can be illustrated by converting Eqn 1 into its untransformed structure using the parameter values from Table 2.1:

$$y_m = 1.238 (y_f + 1)^{0.881} - 1 \quad (2)$$

So if  $y_f$  is e.g. 1, 3 and 5%, the corresponding  $y_m$  values are 1.3, 3.2 and 5.0%, respectively.

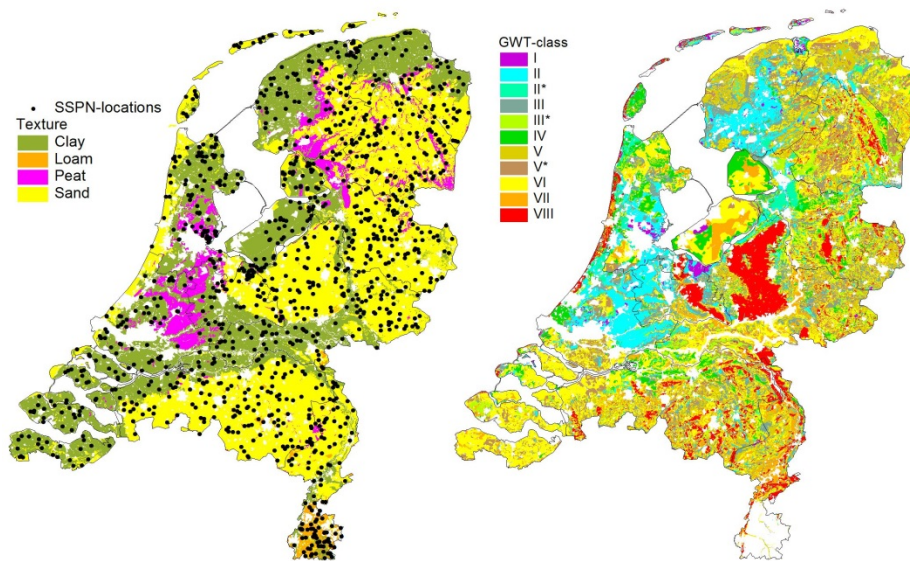
**Table 2.1** Summary of the linear correction regression.

$\alpha_0$	$\alpha_1$	$\sigma_\varepsilon$	$r^2$
0.213	0.881	0.388	0.842

#### *The Netherlands Soil Sampling Program*

The Dutch Soil Information Systems contains the data from the Soil Sampling Program for the Netherlands (SSPN; Finke et al., 2001; Visschers et al., 2007). This dataset contains recent (1998-2001) measurements of soil organic matter at 1210 locations selected using a well-defined stratified random sampling scheme. Measurements were done using loss on ignition (600 °C), which were corrected for clay content using NEN-standard 5754 (2014). Soil map units of the 1:50 000 soil map of the Netherlands, Soil type and groundwater depth classes have been used for stratification

(Figure 2.2). The aim of this stratified sampling is to provide estimates for entire stratification units. Within these units typical areas such as the inner dune areas where bulb flowers are grown may be underrepresented possibly causing some bias for these areas.



**Figure 2.2** Sampling locations of Soil Sampling Program for the Netherlands. Soil type (left-hand side) and groundwater depth class (right-hand side).

As mentioned above, the new map of soil organic matter is based on a trend model in combination with interpolation of the residuals of this trend model. For the trend part of the model, only the data from the Soil Sampling Program for the Netherlands were used because this dataset represents the variability within Dutch soils and because it contains measured organic matter contents. For the interpolation of organic matter content nearly 770 thousand predominantly field determinations of organic matter content were available. Note that the interpolation dataset contains preferential sampling and spatial clustering and may thus cause some bias when compared with the stratified-random sample of SSPN used for calibration of the trend. The interpolation dataset was therefore only used to make local adjustments on the calibrated trend model.

### 2.1.2 Covariates for fitting the trend component of the model

The trend component was fitted after a log transformation of the organic matter content  $y$ . This transformation is given by:

$$y^* = \ln(y + 1) \tag{3a}$$

In which:

$y^*$  =  $e^{\text{log-transformed sum of \% organic matter} + 1}$ .

This transformation was done because the focus was on low organic matter contents (where leaching is highest). An additional benefit of the log-transformation is a better resemblance of the frequency distribution of the transformed organic matter content to the Gaussian distribution. Log organic matter content  $Y^*$  at point  $s$  and depth  $d$  is predicted on the basis of latitude ( $Z$ ), soil physical unit ( $U$ ), soil horizon ( $H$ ), land-use category ( $L$ ) and topsoil texture ( $T$ ) according to:

$$y^*(s, d) = \beta_1 x_1(s) + \beta_2 x_2(s, d) + \delta(d) \beta_3 x_3(s) + \varepsilon_t(s, d) \tag{3b}$$

In which:

$y^*(s, d)$  = predicted  $e^{\text{log transformed organic matter content}}$  at site  $s$  and depth  $d$



---

$x_1$  = northing at location  $s$  (m)

$\beta_{1,2,3}$  = regression coefficients

$x_2(s,d)$  = qualitative variable representing combinations of soil textural class, depth (topsoil or subsoil) and horizon codes at location  $s$  and depth  $d$

$x_3(s)$  = qualitative variable representing combinations of soil texture and land use at location  $s$

$\delta(d)$  = indicator function for the effect of land use on the organic matter content in the topsoil

The indicator function  $\delta$  is given by:

$$\delta(d) = \begin{cases} 1 & \text{if } d \leq 0.15 \text{ m} \\ 0 & \text{if } d > 0.15 \text{ m} \end{cases} \quad (3c)$$

$\varepsilon_t(s, d)$  = residual

An overview of the combinations for  $x_2$  and  $x_3$  is given in Tables 2.2 and 2.3, respectively.

The spatial trend of  $y^*$ , i.e. the expected <sup>e</sup>log-transformed soil organic matter content in 3D space ( $s,d$ ) is determined by three parameter dependent terms: the second term in Eq. 3b depends on the northing in the Dutch coordinate system, the third term consists of a predictor based on combinations of soil physical units and horizon-codes and the fourth term consists of a predictor based on combinations of topsoil texture and land use, i.e. grassland land use or arable land use. The coefficient  $\beta_1$  is calculated to be 5.963e-07. It should be noted that the fourth term is only valid for the prediction of the organic matter content in the topsoil layer. The mapped soil type was obtained by overlaying the Dutch soil map 1:50 000 with the 1210 observation locations of the Soil Sampling Program of the Netherlands. For each soil type, characteristics were obtained from 330 reference profiles as reported by De Vries (1999). Because only 1210 locations with soil organic matter measurements are available to characterize soil units, generalized soil types derived based on the building block of the Staring Series (sandy soils, clayey soils, loamy soils and organic soils) and horizon code (C-horizon versus all other horizons). For each of these soil layers, the mean log-transformed organic matter content was estimated. These mean log-transformed organic matter contents were used as a full-coverage spatial estimate in the interpolation process. Prediction locations are on a regular spaced grid with a spatial-distance of 250 meters and fixed prediction depths of 15 (representing the topsoil layer), 45, 80 and 120 cm.

Notice that the mapped soil type is used for prediction and not the observed soil type. For full coverage prediction this is necessary since only the mapped soil types are exhaustively available while observed soil types are only known at the observation locations. Predictions for the different land use categories (i.e. grass and arable) are made based on the assumption of one uniform land use category occurring over the entire country.

### 2.1.3 Geostatistical interpolation

Three dimensional geostatistical modelling was used, which predicts the value of an attribute  $Z$  that is defined on a horizontal geographical domain ( $S$ ) and vertical depth ( $D$ ) from the soil surface at a point ( $s,d$ ). The prediction function  $Y_p'(s,d)$  is assumed to consist of a trend component in three dimensions representing the 'average' behaviour and a zero-mean residual component correlated in three dimensions (Hoogland et al., 2010; Heuvelink and Griffith, 2010):

$$y_p^*(s, d) = y^*(s, d) + \varepsilon_p(s, d) \quad (4)$$

Here  $y^*(s,d)$  is a structural component representing large-scale variation and  $\varepsilon_p(s,d)$  is a stochastic component representing small-scale, noisy variation. A step-wise trend, where steps are coupled to categorical predictors is used for the part of  $y$  that can be explained by auxiliary information from full-spatial covariates taken from the generalized soil map, recorded land-use and northing (Eqn. 3b). The trend model is used to predict log-transformed soil organic matter contents at all prediction locations and depths. The residual  $\varepsilon_p(s,d)$  contains information on spatial autocorrelation in three-dimensional space. The experimental and modelled autocorrelation of the residuals used in the interpolation procedure are characterized using 3D-variography in a similar manner as reported by Heuvelink and Griffith (2010). It is hereby assumed that the zero-mean stochastic residual  $\varepsilon_p(s,d)$  is multivariate normally distributed. Under appropriate stationarity assumptions, an experimental space-depth

semivariogram may be obtained from the measurements by computing the experimental semivariogram  $\gamma(h_S, h_D)$  as follows:

$$\gamma(h_S, h_D) = \frac{1}{2N(h_S, h_D)} \sum_{i=1}^{N(h_S, h_D)} (\varepsilon(h_S, -s, h_D - d) - \varepsilon(s, d))^2 \quad (5)$$

where  $h_S$  and  $h_D$  are the  $S$  and  $D$  lags and where  $N(h_S, h_D)$  is the number of pairs in the  $S, D$ -domain. Fitting a model to the  $S, D$  experimental semivariogram has some additional problems, due to the distinct differences between the  $S$  and  $D$  variation. For this reason, Bilonick (1988) proposed a model that separates the spatial and depth component (see Hoogland et al. (2010) for details):

$$\gamma(h_S, h_D) = \gamma(h_S) + \gamma(h_D) \quad (6)$$

The experimental space-depth variogram model was fitted by means of differential evolution (Storn and Price, 1997). The implementation of this algorithm in the R-package "DEoptim" (Mullen et al., 2011) was used. The following combined space-depth exponential variogram was fitted, because this model best fits the data and is commonly used (Goovaerts, 1997):

$$\gamma(h_S, h_D) = \gamma_n(h_S, h_D) + \gamma_p(h_S)(1 - e^{-\frac{h_S}{r_S}}) + \gamma_p(h_D)(1 - e^{-\frac{h_D}{r_D}}) \quad (7)$$

where  $\gamma_n(h_S, h_D)$  is the nugget variance,  $\gamma_p(h_S)$  is the partial spatial sill,  $r_S$  is the spatial range parameter,  $\gamma_p(h_D)$  is the partial depth sill, and  $r_D$  is the depth range parameter. Depth ranges are in centimetres below the soil surface and spatial ranges are in meters. The nugget variance  $\gamma_n(h_S, h_D)$  represents short distance variation. It is for instance due to measurement error and variation at distances smaller than the smallest lag distances  $h_S$  and  $h_D$ . The sill variance, *i.e.*, the sum of the nugget variance and the partial sills is the maximum variance attained for locations that are an infinite distance apart. The range parameter is proportional to the maximum distance where locations are still spatially dependent<sup>1</sup>.

#### 2.1.4 Validation procedures

The 1210 locations of the Netherlands Soil Sampling Program were used for validation because they were collected using a well-defined stratified-random sampling scheme allowing for design-based estimation of validation statistics (Brus et al., 1996; De Gruijter et al., 2006). Notice that these locations have been used for fitting the trend model but not for interpolation. For this reason, a cross-validation was carried out in which one data point was left out from the training set and the prediction at this point was validated ("leave one out cross validation", Goovaerts, 1997). This procedure was repeated 1210 times (*i.e.* the number of locations for validation).

The estimation of validation statistics uses the relative area ( $a_s$ ) of each of the  $k$  strata ( $s$ ) from the stratified sampling scheme and the estimated target validation statistic:

$$\hat{T} = \sum_{s=1}^k a_s \hat{T}_s \quad (8)$$

Here the estimated target validation statistic  $T_s$  is based on the differences between predicted ( $\hat{y}(s_i)$ ) and the measured log-transformed organic matter content ( $y(s_i)$ ) at each of the  $s_i$  validation locations within a single stratum  $s$ . The mean error ( $ME$ ) or bias within a single stratum is assessed with the equation:

$$ME = \frac{1}{n} \sum_{i=1}^n (y(s_i) - \hat{y}(s_i)) \quad (9)$$

<sup>1</sup> Note that the range parameter of an exponential model is not equal to the range itself (see *e.g.*, Goovaerts, 1997, p. 88-89). For an exponential model, one often speaks about a practical range. This is the lag distance where the semivariance reaches 95% of its sill value. The practical range is three times the range parameter.

The root mean square error (RMSE) or accuracy within a single stratum is estimated with the equation:

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^n (y(s_i) - \hat{y}(s_i))^2} \quad (10)$$

## 2.2 The new soil organic matter map for the Netherlands

### 2.2.1 The trend model

As described in Section 2.1.2, the trend model was based on a generalised schematisation of Dutch soil types. Because the trend model is based only on observations at 1210 locations obtained using stratified random sampling scheme only a limited number of generalized soil units was used, i.e. 7. Due to the lack of sufficient observations in loamy subsoils, caused by its limited extent, this unit was merged with the sandy subsoil unit. Each of these generalised soil units was coupled to a soil map unit on the Dutch soil map (de Vries, 1999), so that it is possible to create a full-coverage map of organic matter. The soil building blocks associated with each generalised soil unit are listed in Table 2.2.

**Table 2.2** The soil physical building blocks (Staring Series building blocks) for each generalised soil unit.

Generalised soil units	Soil physical building blocks
Sand topsoil	B1,B2,B3,B4,B5,B6
Clay topsoil	B7,B8,B9,B10,B11,B12
Loam topsoil	B13,B14
Peat topsoil	B15,B16,B17,B18
Sand subsoil	O1,O2,O3,O4,O5,O6,O7,O14,O15
Clay subsoil	O8,O9,O10,O11,O12,O13
Peat subsoil	O16,O17,O18

In the overlay of SSPN-data and generalised soil units 9 soil layer types were distinguished, a soil layer type being a combination of a generalised soil unit and a horizon type (C-horizon or All but C-horizon). Five of the fourteen possible combinations of generalised soil units and horizon type do not occur. These are the four combinations of a C-horizon with sand, loam, clay and peat topsoil and the combination of other horizons with a peat subsoil. The mean log-transformed organic matter contents of each soil layer type included in the predictor  $x_2$  in Eqn. 3b are significant and specify the effect of soil layer type on the organic matter content (Table 2.3).

In addition, three land use types, i.e. arable land, pasture (grass), and other (e.g. nature), were distinguished to describe the effect of the texture of the top soil layer (clay or all but clay) on the coefficient  $\beta_3$ .

Predictor  $x_2$  and  $x_3$  are qualitative variables (see Tables 2.3 and 2.4). In the regression, qualitative variables are (automatically) replaced by indicator variables. An indicator variable equals 1 if an observation belongs to a specific soil texture unit and horizon (i.e. a row in Table 2.3) or a specific combination of top soil texture and land use (i.e. a row in Table 2.4), and equals 0 otherwise. Hence, the regression coefficient  $\beta_2$  denotes the (additive) contribution of a specific soil texture unit/horizon class and the regression coefficient  $\beta_3$  denotes the (additive) contribution of a specific combination of top soil texture unit and land use. These contributions will be added to the intercept of the model.

For example, the regression coefficient of a C-horizon in the subsoil consisting of clay is 0.914. This means that it adds 0.914 log-transformed organic matter units to the intercept. Its standard error (7.51E-02) is very small. The 95%-confidence interval constructed from this standard error does not

contain the value zero. Hence, the coefficient is significantly different from zero. This is true for all coefficients in Table 2.3.

**Table 2.3** The effect of the generalised soil unit – horizon combination on the coefficient  $\beta_2$ . *se*  $\beta_2$  are the standard errors of  $\beta_2$ .

Generalised soil unit	Horizon	Coefficient $\beta_2$	S.e. $\beta_2$
Clay, topsoil	All but C-horizons	0.373	1.27E-01
Clay, subsoil	All but C-horizons	0.761	1.32E-01
Clay, subsoil	C-horizon	0.914	7.51E-02
Sand, topsoil	All but C-horizons	0.907	8.48E-02
Sand, subsoil	All but C-horizons	0.859	7.53E-02
Sand, subsoil	C-horizon	0.417	7.14E-02
Loam, topsoil	All but C-horizons	0.957	1.23E-01
Peat, topsoil	All but C-horizons	1.832	1.15E-01
Peat, subsoil	C-horizon	2.745	7.98E-02

Observations in the Soil Sampling Program for the Netherlands showed that soil organic matter content is generally higher in topsoil under grassland than in arable top soils. This is confirmed in the regression analysis, which showed higher coefficients for grassland soils than for arable soils (Table 2.4). The regression analysis also showed that the effect of land-use was different in clay top soils than in other (predominantly sandy) top soils. For this reason, different coefficients were determined for clay soils than for other soils. Notice that the correction was only applied to the top soil (i.e. 15 cm depth) because the effect of land-use on soil organic matter content in deeper soil horizons appeared limited.

**Table 2.4** The effect of soil texture and land-use on coefficient  $\beta_3$ .

Top soil texture	Land-use	Coefficient $\beta_3$	S.e. $\beta_3$
All but clay	Arable	0.299	8.43E-02
Clay	Arable	0.665	1.21E-01
All but clay	Grass	0.485	6.56E-02
Clay	Grass	1.245	1.04E-01
All but clay	Other (e.g. nature)	0.291	6.19E-02
Clay	Other (e.g. nature)	0.928	1.31E-01

The additional effect of the northing on organic matter was obtained by linear regression and incorporated in the trend model as  $\beta_1$ . This indicates that in the same soil type, organic matter is significantly higher in the North of the country than in the South. The predicted gradient in the organic matter content is shown in Table 2.5. A North – South trend in organic matter is often observed at a larger (continental) spatial scale (e.g. Tiktak et al., 2004; 2013). Only the effects on soil organic matter content that are not accounted for by the spatial variation in soil units are incorporated in the coefficient for latitude.

**Table 2.5** North – South gradient in predicted organic matter content in top layer of sandy and clay soils with land use arable land and grassland.

Location	Soil type	% Organic matter	
		arable	grass
North	sand	3.83	4.81
South	sand	3.05	3.88
North	clay	3.06	6.26
South	clay	2.39	5.06

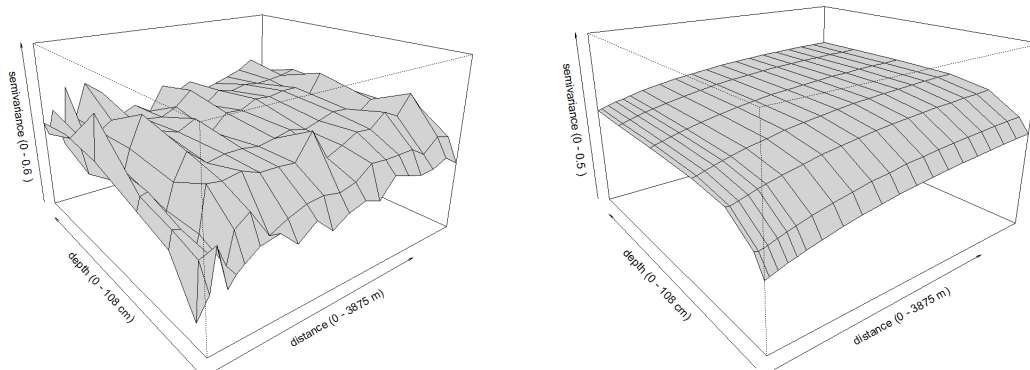
## 2.2.2 Three dimensional variography

For the interpolation, all observations (including corrected field-estimates, but excluding SSPN data) were used. The averaged difference between residuals of log-transformed soil organic matter contents were calculated for space- and depths-lags according to Eqn. 5 for each pair of observations. Three-dimensional plots of the experimental semi-variance and the modelled semi-variance (Eqn. 7) are shown in Figure 2.3.

The parameters of the fitted semi-variogram model (Eqn. 7) used in the interpolation procedures for the log-transformed organic matter contents are given in Table 2.6. The semi-variogram of the log-transformed residuals of organic matter content shows structure, indicating spatial autocorrelation depending on horizontal and vertical distances. In the vertical direction, the largest variation is present indicated by the higher sill variance with depth compared to the horizontal spatial sill.

**Table 2.6** Fitted variogram models

Variogram model	$\gamma_n(h_S, h_D)$	$\gamma_p(h_S)$	$r_S(m)$	$\gamma_p(h_D)$	$r_D(cm)$
Log-transformed y	0.160	0.100	1500	0.120	10

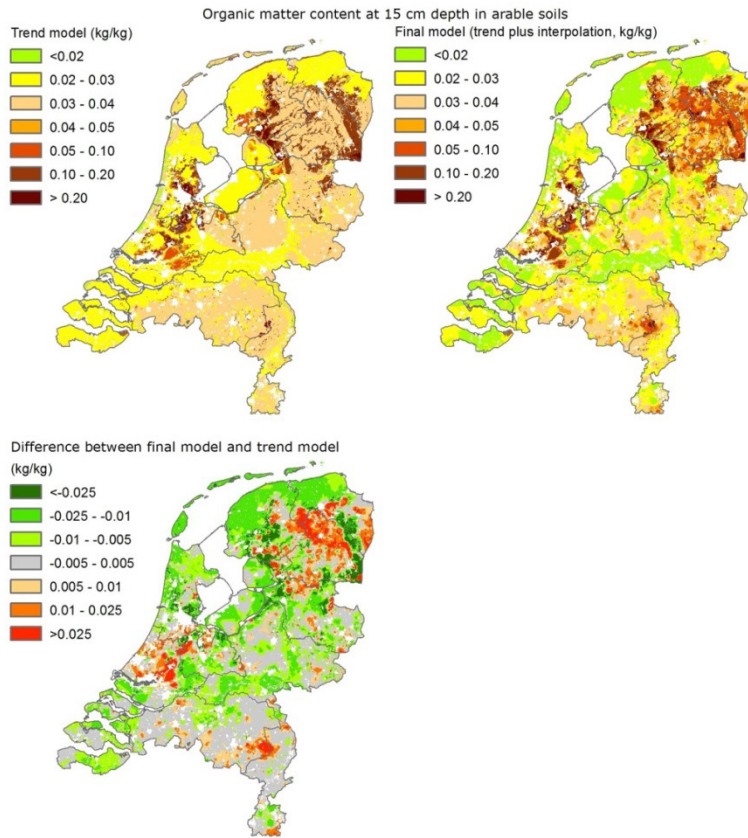


**Figure 2.3** Experimental (left) and modelled (right) semi-variance of residuals of log-transformed organic matter content. Notice that the horizontal and vertical scales are different.

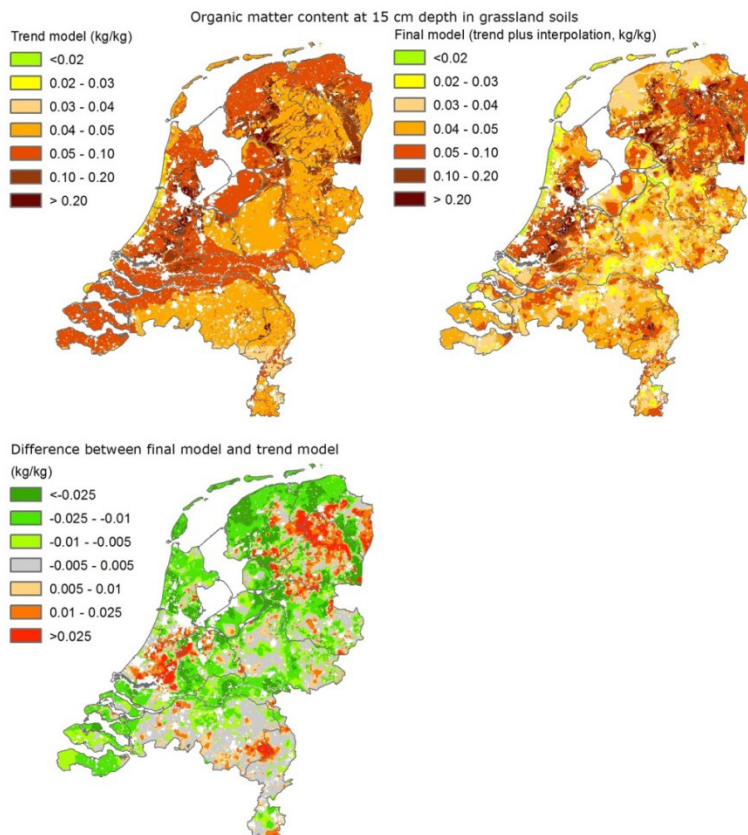
## 2.2.3 Prediction of soil organic matter content

The prediction of log-transformed organic matter content in the trend model is based on average log-transformed organic matter contents for each combination of soil unit, texture and land use. The coefficients of the variogram model in Table 2.6 were used for interpolation. The interpolation procedure takes into account the quantified prediction error of the corrected field determinations from the correction regression (Table 2.6). Local interpolation was performed using the nearest 100 observations defined with the variogram-distance. This implies that only the 100 locations with the lowest semi-variance according to the fitted variogram model were used.

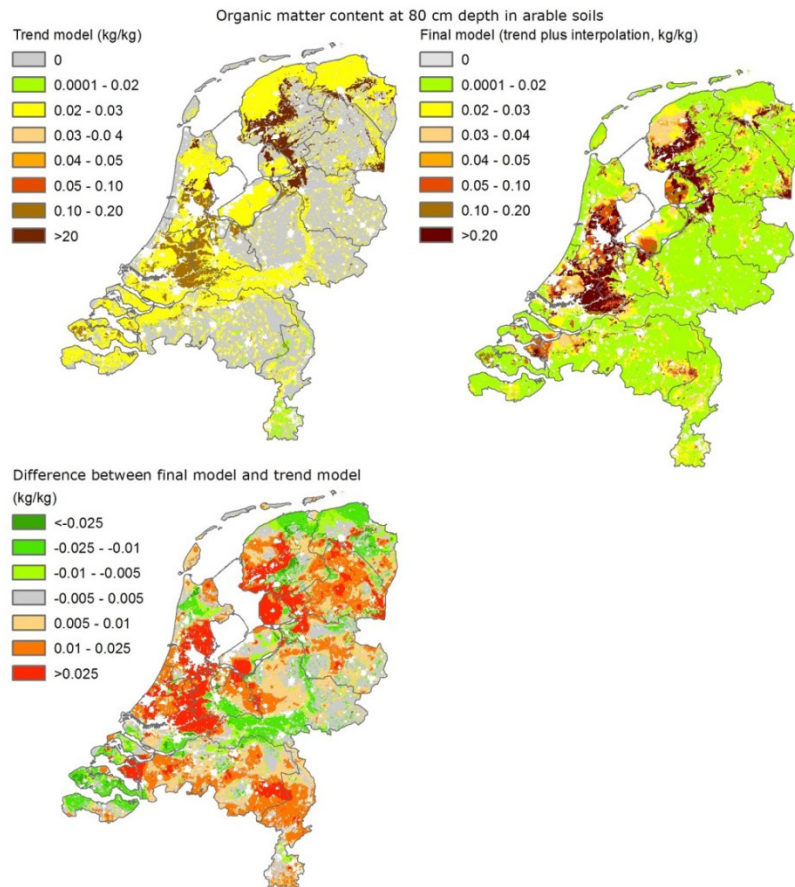
Results of the trend model for a depth of 15 cm in arable soils are shown in Figure 2.4. Based on the trend model only, the organic matter content in the top soil of areas with a clayey topsoil, such as the Southwest of the Netherlands and the Northern part of the Groningen and Friesland Provinces, are mostly in the range of 2 to 3%. For the top layer in areas with sandy soils, for example in the Noord-Brabant and Gelderland Provinces, the predicted soil organic matter using the trend model mostly ranges from 3 to 4%. The subsequent interpolation procedure resulted in a substantial decrease in the organic matter content of the clayey soils in the South-West of the Netherlands. For areas with peaty soils in Central Holland and sandy soils on bolder clay in Drenthe Province, the interpolation procedure resulted in an increase in the organic matter content. Results of the trend model for a depth of 15 cm in grassland soils are shown in Figure 2.5. The interpolation for these soils resulted in a similar decrease for clayey top soils and in an increase of the organic matter content in soils with peaty top soil layers in Central Holland. In Figure 2.6 the results are shown for the subsoil layer 60 – 100 cm.



**Figure 2.4** Predicted organic matter content (kg/kg) at 15 cm of arable soils using the trend model only (top left), the final model (trend plus interpolation, top right) and the differences in the predicted organic matter content (final minus trend, bottom).



**Figure 2.5** Predicted organic matter content (kg/kg) at 15 cm of grassland soils using the trend model only (top left), the final model (trend plus interpolation, top right) and the differences in the predicted organic matter content (final minus trend, bottom).



**Figure 2.6** Predicted organic matter content (kg/kg) at 80 cm of arable soils using the trend model only (top left), the final model (trend plus interpolation, top right) and the differences in the predicted organic matter content (final minus trend, bottom).

#### 2.2.4 Comparison with data from Reijneveld et al. (2009)

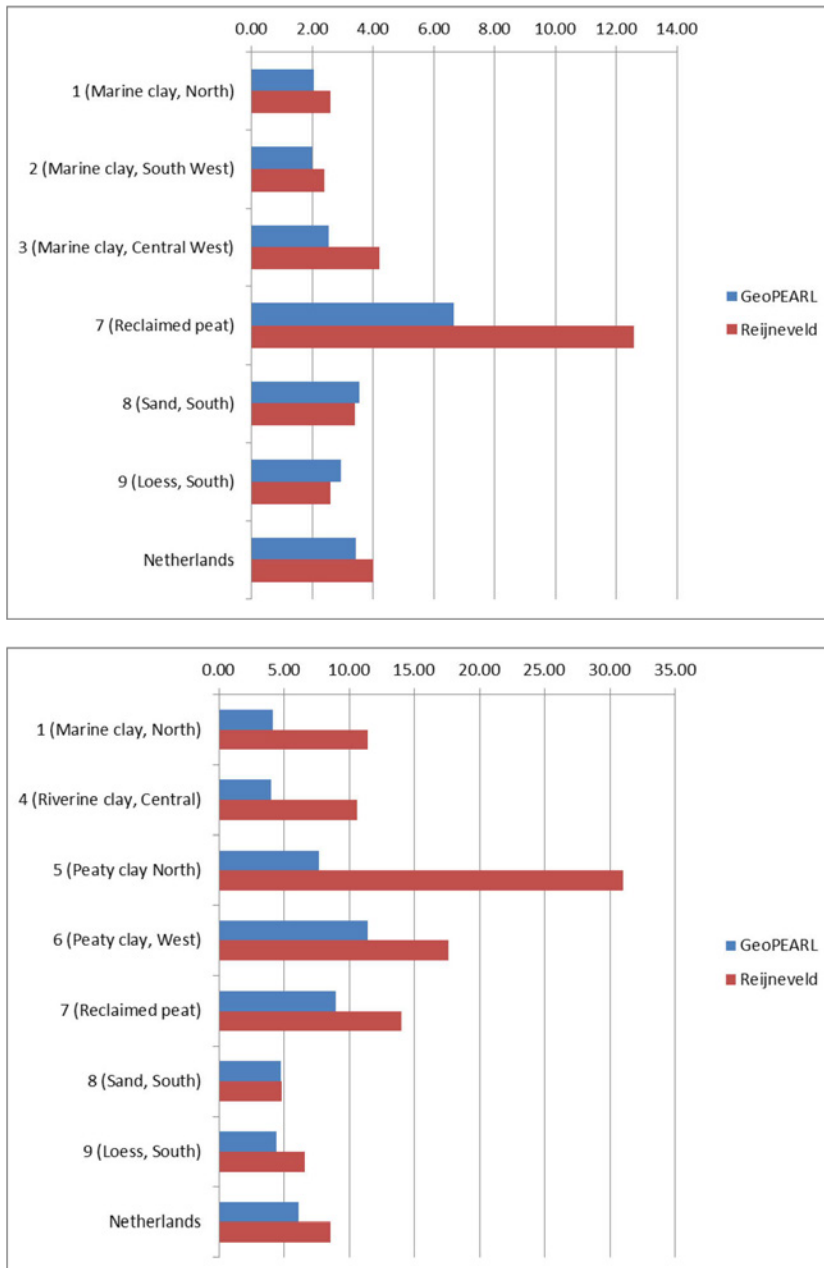
Reijneveld et al. (2009) determined soil organic carbon contents of agricultural land based on some 2 million samples from farmer's fields. They distinguished nine regions, which are based on soil texture and land-use (arable land and permanent grassland). Because of the vast amount of observations in this dataset, it can be seen as a reference. So we compared their measurements with the data in the SSPN-dataset (Figure 2.7). This table shows that the mean organic matter content of topsoils in arable land is comparable for both datasets. So the use of the SSDN-dataset (consisting of measurements at 1 210 locations) for creating the trend model is considered justified.

It should be noted that measurements by Reijneveld et al. (2009) could not be compared directly for the reasons below. First measurements by Reijneveld et al. (2009) were carried out in the period 1984-2004 using two different methods. In mineral soils, soil organic carbon contents were determined using the wet oxidation method proposed by Walkley and Black (1934). From 1994 onwards, soil organic carbon contents were determined using dry combustion at 600 °C. Dry combustion gives a good estimate of organic C for non-calcareous soils. Indeed, Sleutel et al. (2007) showed a good correlation between both methods (coefficient 1.013,  $r^2 = 0.99$ ) for soils in Flanders. We therefore considered the use of both methods in one dataset justified.

Second, measurements in the SSDN-dataset refer to organic matter contents and measurements by Reijneveld refer to organic carbon. So a conversion factor is needed to convert organic carbon into organic matter. Often in pesticide risk assessments, a factor of 1.724 is used (FOCUS, 2014). However, Reijneveld (2014, personal communication) found a conversion factor of 2.0 based on a dataset of 100 000 simultaneous measurements of organic matter and organic carbon. This factor is comparable to the factor of 1.9 found by Sleutel et al. (2007). Hence, for soils in Flanders and the Netherlands, the conversion factor of 1.724 would underestimate the organic matter content.



The results of the comparison between the Reijneveld data and those predicted in the new soil organic matter map are shown in Figure 2.7. For arable soils the agreement between the predicted new organic matter map and the measurements is fairly good, excepting the reclaimed peat area. As the data of Reijneveld have been collected in the period 1994 – 2004, the effect of oxidation of peat in these soils since then is expected to have resulted in a decrease in the organic matter content for the sites in this area that have been included in the SSDN dataset.



**Figure 2.7** Average organic matter content for the 9 regions in the study of Reijneveld et al. (2009) and the content predicted in these regions for arable land use (top) and grass land use (bottom).

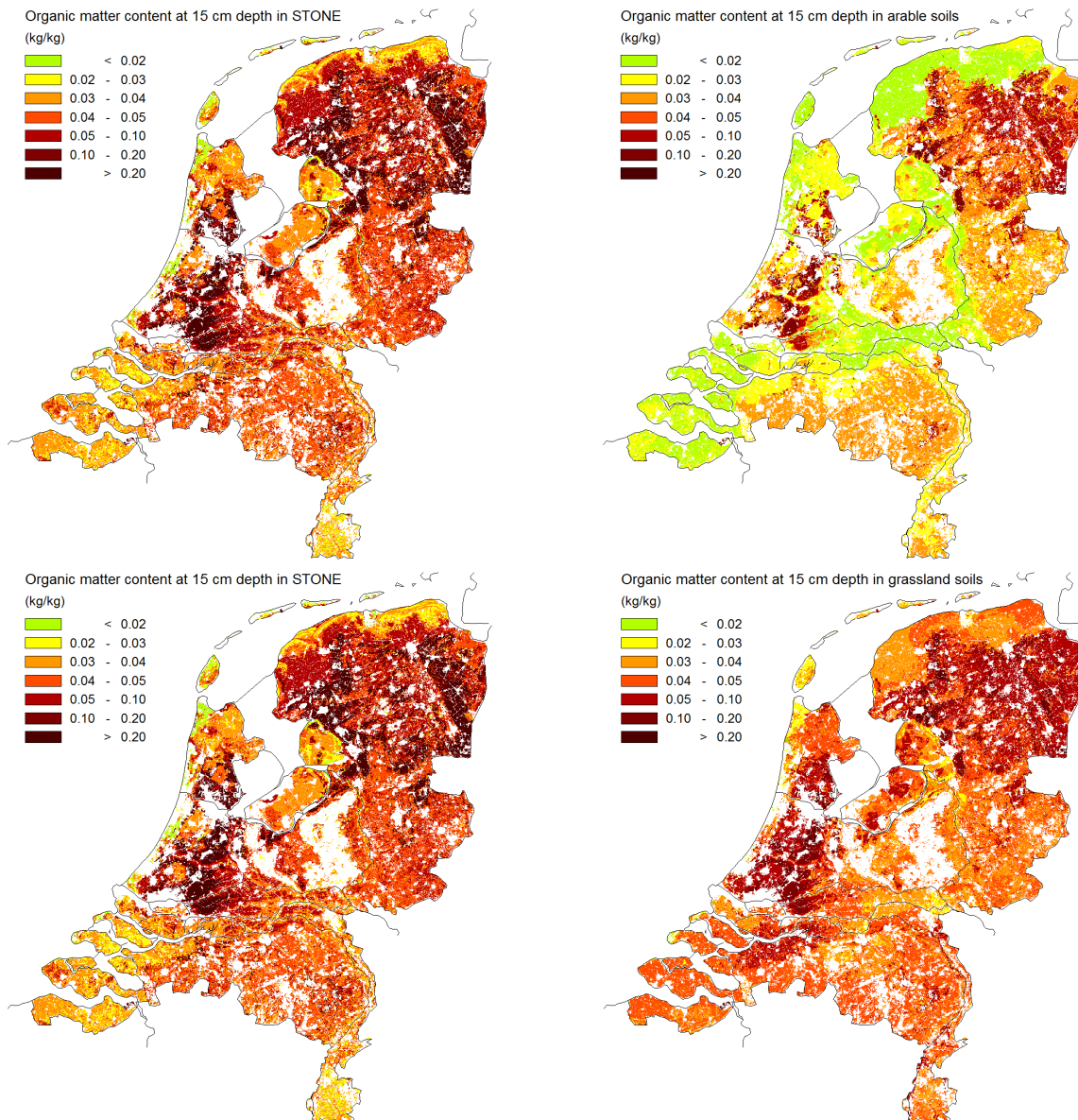
It should be noted that if a factor of 1.724 would have been used for the comparison of the Reijneveld data and the predicted values in the new soil organic matter map, the Reijneveld values would decrease by a factor 0.862. This would decrease the difference for the marine clay regions in the North and the Southwest, but it would increase the difference in the sand and löss regions in the South (see Figure 2.7 top graph). However, the use of a factor of 1.724 cannot be justified, since Reijneveld found a value of 2.0 based on 100 000 measurements.



The difference between the organic matter contents in grassland soils measured by Reijneveld et al. (2009) and the predicted values in the new organic matter map could be explained by the fact that Reijneveld et al. sampled the top 5 cm of the soil, whereas the predictions have been made for a depth of 15 cm.

### 2.2.5 Difference between the new and the old organic matter content map

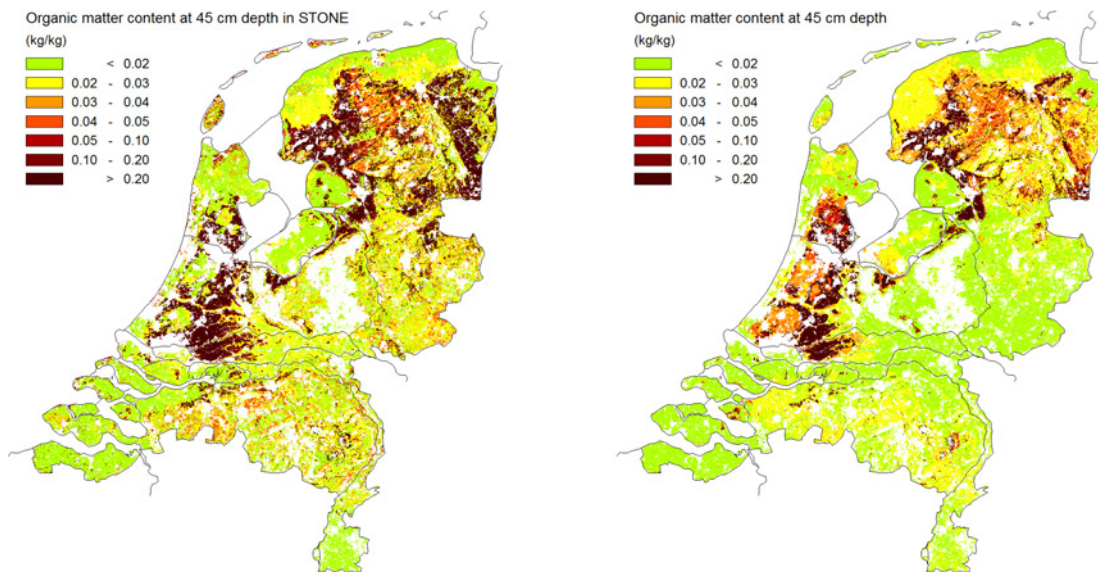
Soil organic matter content in the topsoil of arable land is generally lower in the new map than in the map included in earlier versions of GeoPEARL (Figure 2.8). Organic matter contents in grassland soils are, however, slightly higher.



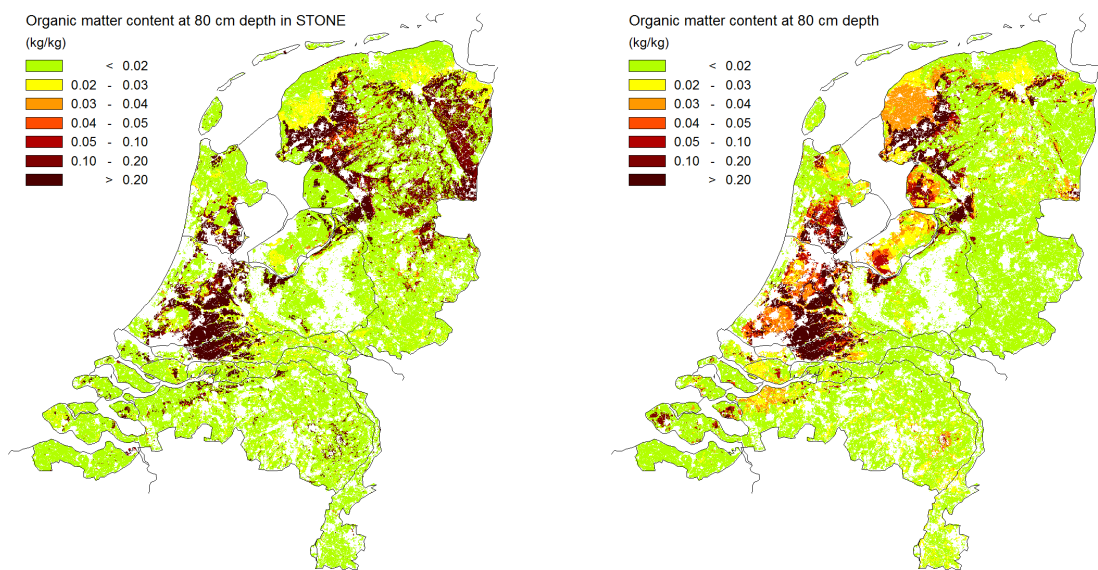
**Figure 2.8** Predicted soil organic matter for the topsoil (0-30 cm) in earlier GeoPEARL versions (left) and predicted organic matter in the new GeoPEARL version (right). The top row shows organic matter for arable soils and the bottom row shows the map for grassland soils.

In the new organic matter content maps, organic matter has lower values in the subsoil layers (30-60 cm, 60-100 cm and 100-140 cm) as well (note that there is no distinction between arable and grass for the subsoil). These results are shown in Figures 2.9 to 2.11. There are remarkable differences for the Northern peat region, which may be due to a combination of two factors, i.e. (i) the fact that higher values are underestimated because of the log-transformation mentioned above, and

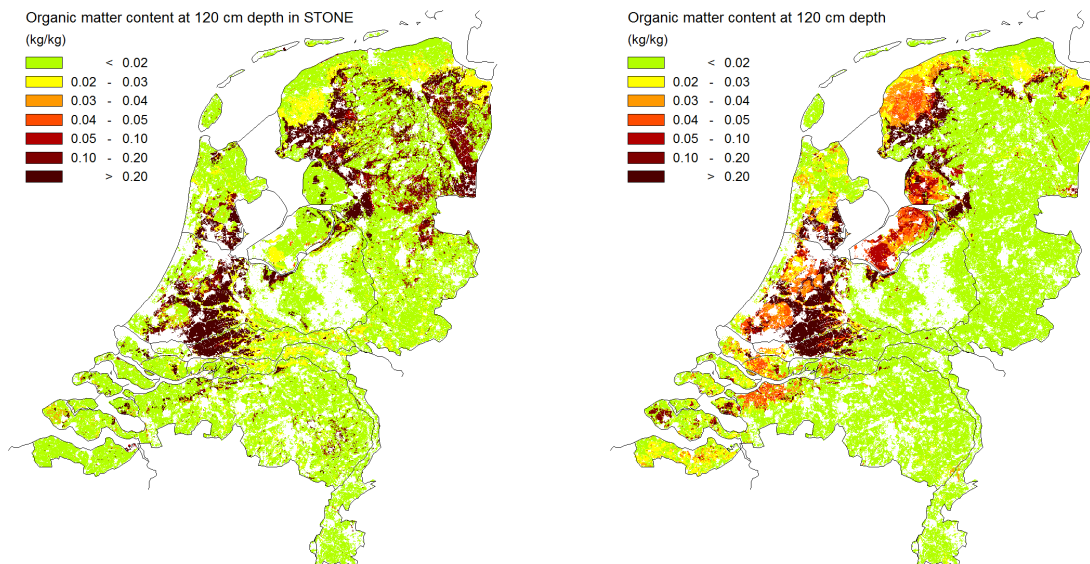
(ii) the fact that peat layers have vanished as a result of drainage and subsequent oxidation of peat (Van den Akker et al., 2008; De Vries et al., 2009). The old GeoPEARL maps were based on a soil map version in which the process of peat oxidation was not yet accounted for (Kempen et al., 2009, Kempen et al., 2015). The new maps also show clay soils where subsoil organic matter content is higher in the new map. This is for example the case in the reclaimed polder areas and in the province of Friesland.



**Figure 2.9** Predicted soil organic matter for the subsoil (30-60 cm) in earlier GeoPEARL versions (left) and predicted organic matter in the new GeoPEARL version (right).



**Figure 2.10** Predicted soil organic matter for the subsoil (60-100 cm) in earlier GeoPEARL versions (left) and predicted organic matter in the new GeoPEARL version (right).



**Figure 2.11** Predicted soil organic matter for the subsoil (100-140 cm) in earlier GeoPEARL versions (left) and predicted organic matter in the new GeoPEARL version (right).

## 2.2.6 Validation of the new and earlier organic matter content maps

Validation of both the new and the earlier organic matter content maps was carried out using the point locations of the Soil Sampling Program for the Netherlands using the procedure in paragraph 2.1.4. As described there, validation was done for four strata of this Sampling Program, i.e. sand, clay, loam and peat soils, covering all land use. Average values of organic matter content of these four strata are shown in Table 2.7.

**Table 2.7** Mean soil organic matter content (%) of the four strata of the Soil Sampling Program for the Netherlands.

Depth (cm)	All strata	Sand	Clay	Peat	Loam
15	5.34	5.20	5.29	21.24	3.29
45	4.29	4.14	4.30	19.50	1.35
80	4.57	2.55	6.32	25.80	1.05
120	4.86	2.12	7.36	24.90	1.03

### Mean error or bias

The mean error of the new map and the earlier map is calculated using Eqn. 9 and is based on the differences between the predicted and measured log-transformed organic matter content within the four strata. Table 2.8 and Table 2.9 show that organic matter contents are systematically too high in the old map and systematically too low in the new map. The absolute difference is, however, smaller in the new map (0.6% in the new map versus 1.5% in the old map).

In sandy soils, the systematic error of the new map is considerably less than in other soil types. Clay and peat soils are generally more heterogeneous than sandy soils. In deeper soil horizons of clay soils, peat layers are commonly found. These peat layers lead to higher observed organic matter contents, but are not present in the soil schematisation. This leads to a high systematic error in deeper horizons of clay soils. Errors are also relatively large in peat soils because of the log-transformation of organic matter (see text below). From a risk assessment point of view, this is however not important because leaching hot-spots are primarily found in regions with low organic matter contents.

**Table 2.8** Mean Error (ME as percentage of organic matter) of the old organic matter content map for each stratum of the Soil Sampling Program for the Netherlands. Negative values indicate that predictions are too high and vice versa.

Depth (cm)	All strata	Sand	Clay	Peat	Loam
15	-1.99	-1.74	-2.38	-0.03	0.50
45	-2.03	-1.26	-2.73	-11.14	0.29
80	-1.75	-2.87	-0.70	-3.93	-0.02
120	-0.37	-1.28	0.61	-7.94	0.42

**Table 2.9** Mean Error (ME as percentage of organic matter) of the new organic matter content map for each stratum of the Soil Sampling Program for the Netherlands. Negative values indicate that predictions are too high and vice versa.

Depth (cm)	All strata	Sand	Clay	Peat	Loam
15	0.26	-0.06	0.48	8.29	-0.49
45	0.34	0.29	0.36	4.35	-0.44
80	0.69	0.12	1.28	2.01	-0.6
120	0.98	-0.01	2.06	-1.79	-0.51

The average bias of 0.6% over all soil types and depths in the new organic matter content map is caused by the log-transformation, which was done to gain higher prediction accuracy at low values. Validation should therefore preferably be done on the log-scale; however, results at that scale cannot easily be interpreted. Table 2.10 confirms that the mean error of log-transformed organic matter contents is generally close to zero and that predictions at log scale are unbiased.

**Table 2.10** Mean Error (ME as percentage of log-transformed organic matter) of the new organic matter content map for each stratum of the Soil Sampling Program of the Netherlands. Negative values indicate that predictions are too high and vice versa.

Depth (cm)	All strata	Sand	Clay	Peat	Loam
15	0.09	0.04	0.14	0.57	-0.04
45	0.04	0.01	0.08	0.23	-0.07
80	-0.04	-0.1	0.01	0.12	-0.09
120	-0.08	-0.12	-0.05	-0.04	-0.04

#### Root mean square error or accuracy

The root mean square error (RMSE) gives an indication of the accuracy of the map. The RMSE value is calculated for each of the strata and prediction depths according to Eqn. 10. The results are given in Tables 2.11 and 2.12. The new map is generally more accurate than the old map.

**Table 2.11** Root Mean Square Error of the old organic matter content map for each stratum of the Soil Sampling Program of the Netherlands.

Depth (cm)	All strata	Sand	Clay	Peat	Loam
15	7.72	5.97	9.08	15.62	1.43
45	11.89	8.98	14.22	20.22	0.72
80	12.18	9.30	14.54	19.38	0.45
120	11.43	8.52	13.89	10.72	0.58



**Table 2.12** Root Mean Square Error of the new organic matter content map for each stratum of the Soil Sampling Program of the Netherlands.

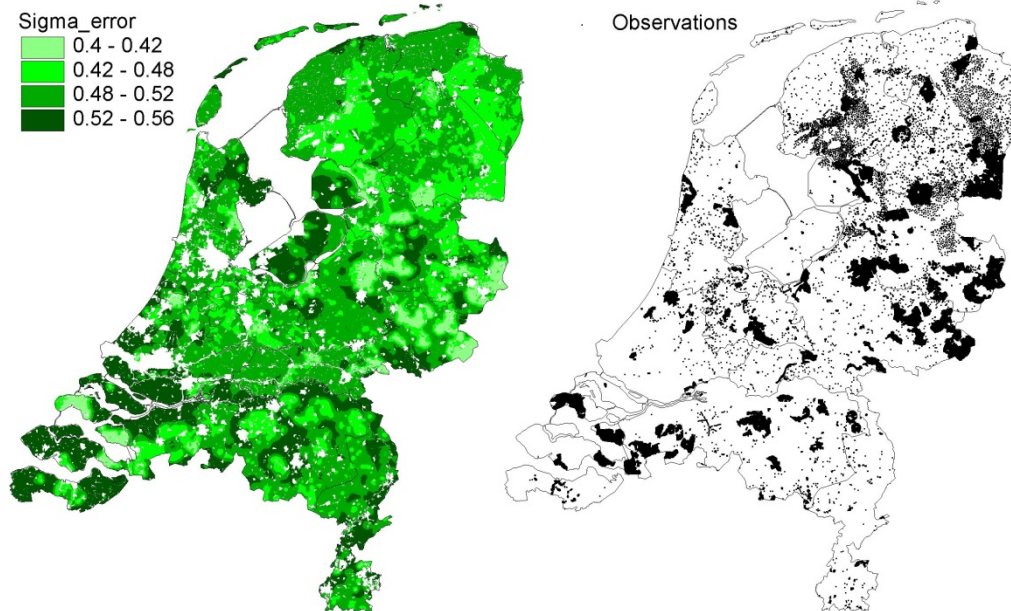
Depth (cm)	All strata	Sand	Clay	Peat	Loam
15	4.05	3.76	3.79	17.52	1.46
45	7.69	8.21	6.99	18.37	1.37
80	9.04	6.60	10.94	15.95	1.38
120	10.76	7.24	13.38	18.21	0.87

### 2.2.7 Model application in specific areas

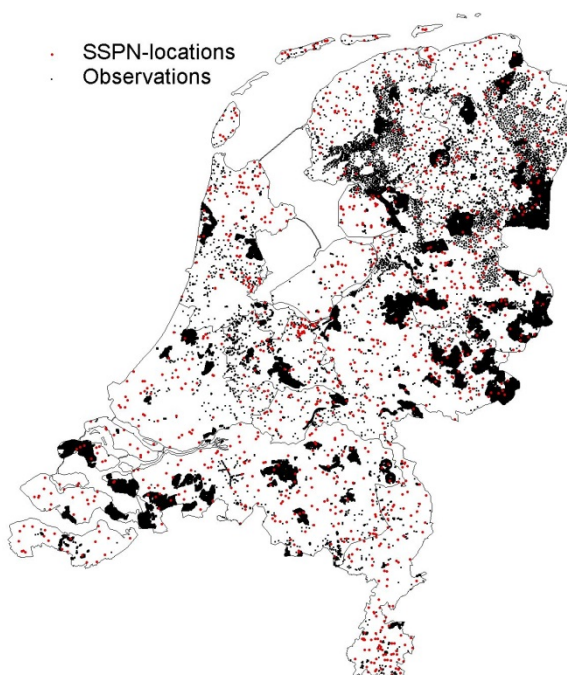
The accuracy of the new organic matter map can be quantified by the variance of the prediction error. Kriging not only gives unbiased predictions (given the data), but also minimizes and quantifies the variance of the prediction error at each prediction point. The square root of the prediction error is given in Figure 2.12. The accuracy of the map is highest in regions with many observations (e.g., Eastern parts of the Netherlands) and lower in regions with less observations (e.g., Flevoland), which is illustrated in the right-hand side of Figure 2.12. From Figure 2.13 it is clear the SSPN-data point are well distributed over the Netherlands, whereas the observation points are very unequally distributed. In the GeoPEARL assessments, plots are selected within the crop area of interest. For the major crops, such as maize, cereals, potatoes and sugar beet, the area of use is large, ranging from 108 000 to 228 000 ha and the effect of the areas with low accuracy can be expected to be counterbalanced by areas with higher accuracy. However, for some crops the area is much smaller, e.g. 18000 ha for flower bulbs and 2200 ha for asparagus. Moreover, the areas of groundwater abstraction areas are also comparatively small and may be located in areas with lower map accuracy. This will result in a greater uncertainty in the outcome of the GeoPEARL assessments. This uncertainty can be reduced by introducing more observations in areas with low accuracy as they become available. By repeating the interpolation step as described in sections 2.2.2 and 2.2.3, a soil organic map with higher accuracy could be achieved.

The model to predict the organic matter content as described in sections 2.1.2 and 2.1.3 was used to calculate the 10, 50 and 90 percentiles of the organic matter content in the top 30 cm of arable soils. A series of 100 simulations (by means of sequential Gaussian simulation, Goovaerts, 1997) were done to obtain 100 realisations of the soil organic matter map for this layer. The organic matter contents corresponding to the 10, 50 and 90 percentiles were calculated for each gridcell centre and the resulting maps are shown in Figure 2.14. In addition, a map is presented in Figure 2.14 on the difference between the P90 and P10 value of the organic matter content. This difference is a measure of the prediction uncertainty of the organic matter content throughout the Netherlands. It should be noted that the map with data on the P50 is similar to the new organic matter map for this layer as presented in Figure 2.4. The map on the difference between the P90 and the P10 shows that this difference is roughly between 3 and 7.5% in regions with sandy soils, e.g. in the Provinces of Noord-Brabant, Gelderland, Overijssel and Drenthe and between 2 and 5% in regions with predominantly clayey soils, e.g. Zeeland and the Northern parts of Friesland and Groningen. The width of the interval between P10 and P90 can be expected to be comparatively large at individual grid cells (point predictions) as shown in Fig. 2.14. From Figures 2.12 and 2.13 it is evident that in areas with a large number of observations the uncertainty in the predicted organic matter content is less than in areas with only few measurements.

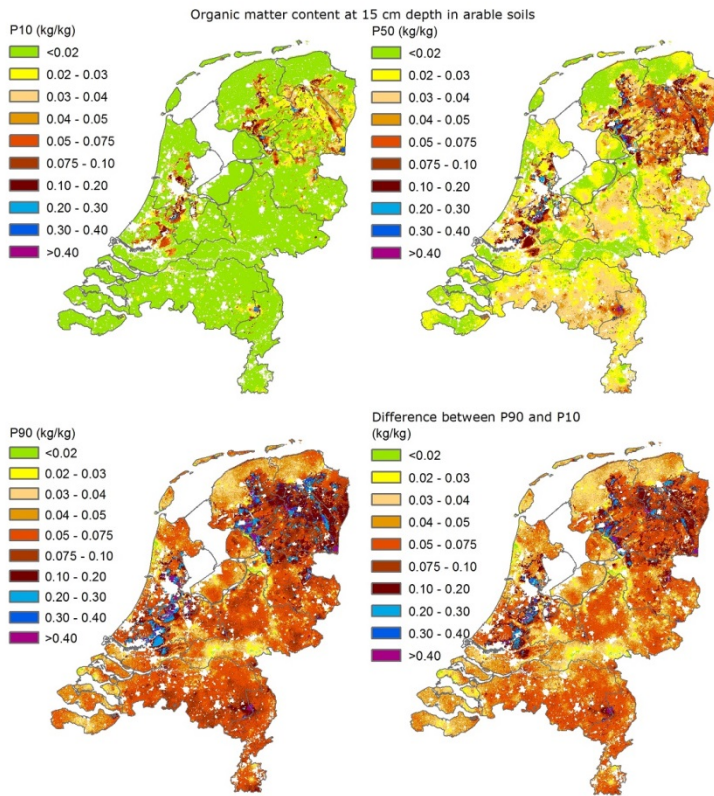
The current version of GeoPEARL does not process data at grid points, but at STONE plots. Each STONE plot consists of several, not necessarily contiguous, grid cells. Given the 100 realisations, the organic matter contents at grid cell centres can be aggregated to STONE plot medians including an estimate of the 10% and 90% percentiles of these STONE plot medians. Due to aggregation, the uncertainty of the STONE plot medians, as expressed by the difference between the 90% and 10% percentiles is greatly reduced. This is exemplified in Figure 2.15, which shows the same results as Figure 2.14, but then for STONE plots instead of grid cell centres. Intuitively, this makes sense, as prediction at grid cell centres is much more ambitious than predicting a single summary statistic (like the median) for larger areas. This important effect of spatial aggregation on prediction accuracy has also been clearly illustrated by McBratney and Webster (1981).



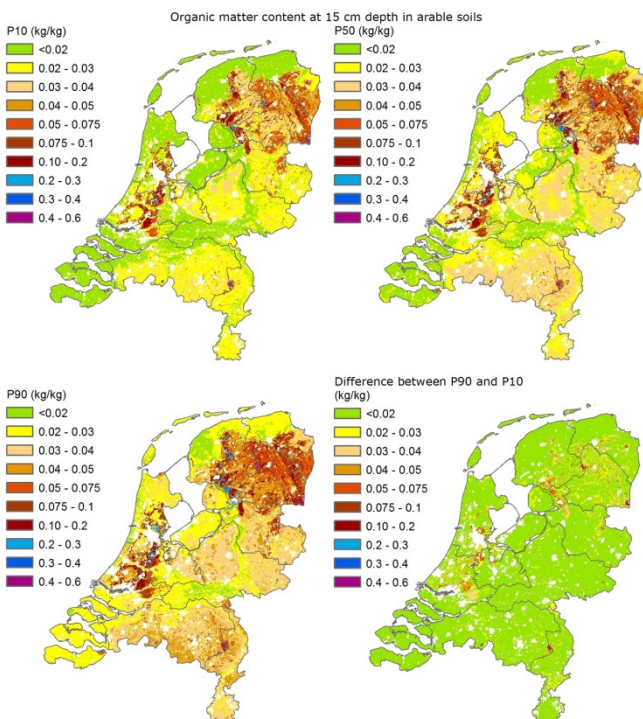
**Figure 2.12** Map of the standard deviation of the prediction error (left graph) and map of observation points (right graph). Higher values of *Sigma\_error* imply lower map accuracy and lower values imply higher map accuracy. Observations indicated by dots.



**Figure 2.13** Map of observation points (black dots) and the SSPN locations (red dots).



**Figure 2.14** Maps of the 10 (top left), 50 (top right) and 90 (bottom left) percentile of organic matter contents and the map of the difference of the 90 and 10 percentiles (bottom right) of organic matter content in the top 30 cm in arable soils.



**Figure 2.15** Maps of the 10 (top left), 50 (top right) and 90 (bottom left) percentile of organic matter contents in STONE plots and the map of the difference of the 90 and 10 percentiles (bottom right) of organic matter content in the top 30 cm in arable soils in these plots.

# 3 Schematisation of GeoPEARL using the new organic matter map and calculations with GeoPEARL

## 3.1 Modifications in the soil schematisation

### 3.1.1 Modifications of organic matter contents in soil profile descriptions

In the current soil schematisation of GeoPEARL (version 3.3.3) 456 soil profiles have been identified. In order to correct the organic matter contents in these soil profiles, the median organic matter content has been calculated for each depth considering only the grid cells that are linked with a specific soil profile.

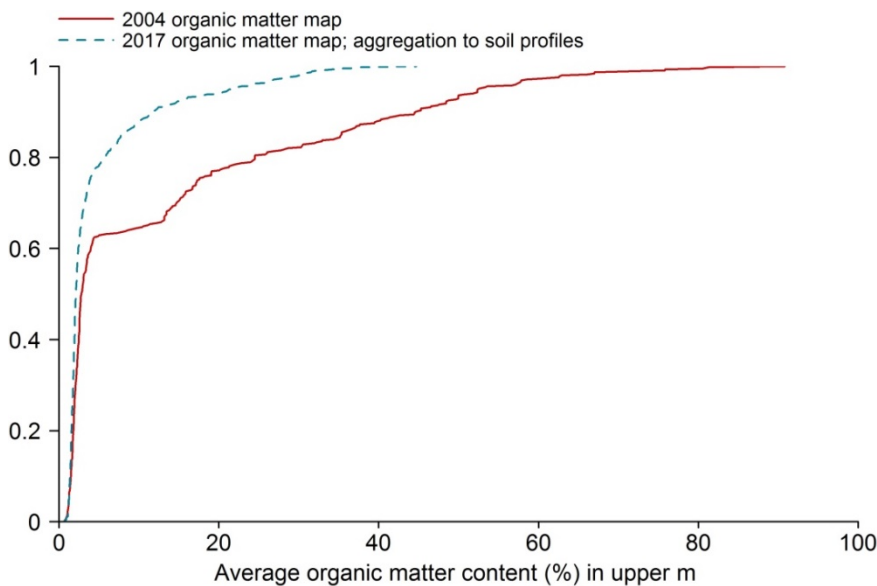
The layers for which the organic matter content has been estimated do not fully match the layers as they have been defined in the current soil schematisation. Organic matter contents have been calculated for a depth of 0.15 m (layer 0 – 0.3 m), 0.45 m (layer 0.3 – 0.6 m), 0.80 m (layer 0.6 – 1.0 m) and 1.2 m (layer below a depth of 1.0 m).

Layer number 5 has a thickness of 0.10 m and this layer extends from 0.25 to 0.35 m. This layer is not fully part of one of the four layers for which the new values have been obtained. Therefore, this layer has been split and the layer from 0.20 – 0.30 m has been assigned to layer number 4. In addition, the thickness of layer number 9 has been modified, so the bottom boundary in the new discretisation is now at a depth of 1.0 m. This modification has no consequences, because the properties of the layers 9, 10 en 11 being identical. An overview of the changes in the discretisation is given in Table 3.1.

**Table 3.1** Discretisation of the soil profiles in the GeoPEARL schematisation.

Layer-number	GeoPEARL 333			GeoPEARL 444			
	Thickness (m)	Depth (m)	ContentId	Thickness (m)	Depth (m)	ContentId	Depth new o.m. map (m)
1	0.05	0.05	1	0.05	0.05	1	0.15
2	0.1	0.15	2	0.1	0.15	1	0.15
3	0.05	0.2	3	0.05	0.2	1	0.15
4	0.05	0.25	3	0.1	0.3	1	0.15
5	0.1	0.35	4	0.05	0.35	2	0.45
6	0.15	0.5	5	0.15	0.5	2	0.45
7	0.1	0.6	6	0.1	0.6	2	0.45
8	0.15	0.75	7	0.15	0.75	3	0.8
9	1	1.75	8	0.25	1	3	0.8
10	0.25	2	8	1	2	4	1.2
11	11	13	8	11	13	4	1.2



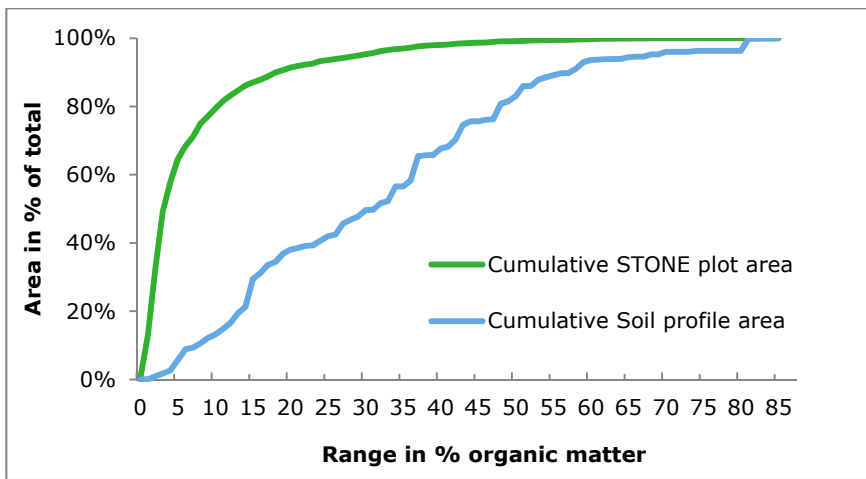


**Figure 3.1** Cumulative frequency distribution of the organic matter content in the upper *m* of the soil profile using the 2004 (solid line) and the 2017 (dashed line) soil organic matter map of GeoPEARL.

The frequency distribution of the organic matter content in the upper metre of the soil based on the aggregation on soil profile basis for the old and the new soil schematisation is shown in Figure 3.1. For the range of low organic matter contents the difference between the 2 schematisations is small. As the spatial 90 percentile of the leaching concentration can be expected to be linked to a soil profile with a soil organic matter in this lower range, the effect of the change to this schematisation on the target leaching concentration is likely to be limited.

### 3.1.2 Modifications of organic matter contents in plot descriptions

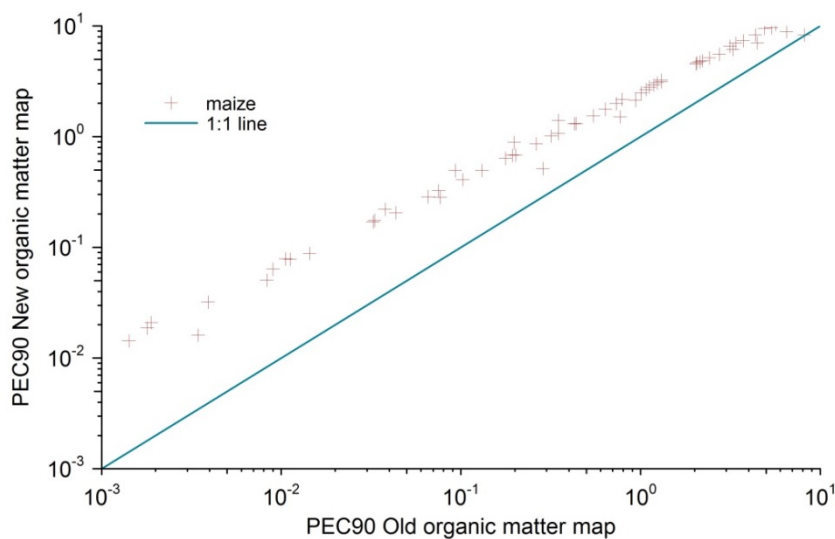
Because the aggregation to a total of 456 different organic soil profiles results in a lower spatial resolution of the soil organic matter map, another aggregation method was applied. Using this method the median organic matter content has been calculated for each depth considering only the grid cells that are linked with a specific STONE plot. As the total number of STONE plots is 6405, a total of 6405 soil organic matter profiles were obtained. For both aggregation methods, the cumulative area was plotted against the range in organic matter content. From the results as shown in Figure 3.2 it is evident that the soil profile areas are much more heterogeneous than the STONE plots. For the STONE plots, 50% of the area has a range between the minimum and the maximum organic matter content of less than 3%. For soil profile areas, only 3% of the area has a organic matter range less than 3%. Therefore, the aggregation on the STONE plot basis was selected to obtain a new soil schematisation.



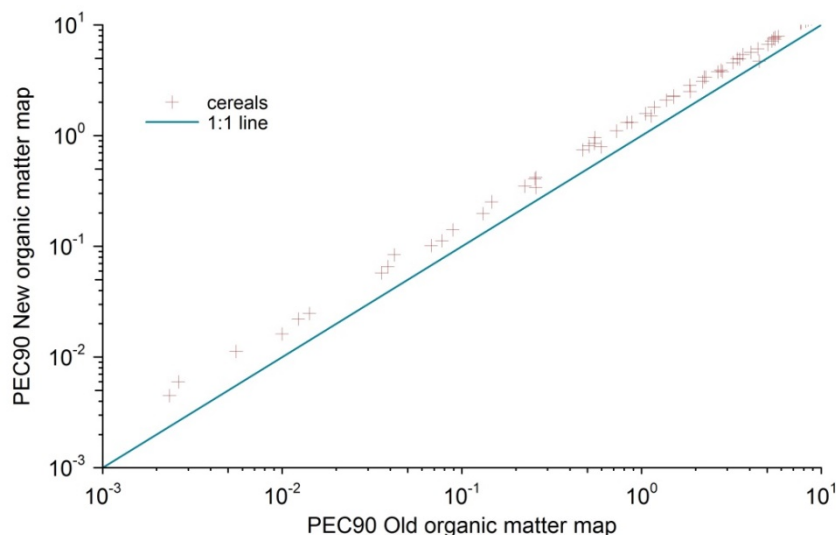
**Figure 3.2** Range in organic-matter contents (difference between maximum and minimum) at a depth of 15 cm using an aggregation to soil profiles (465 soil profiles) en STONE plots (6405 plots).

### 3.2 Calculations using GeoPEARL version 4.4.4

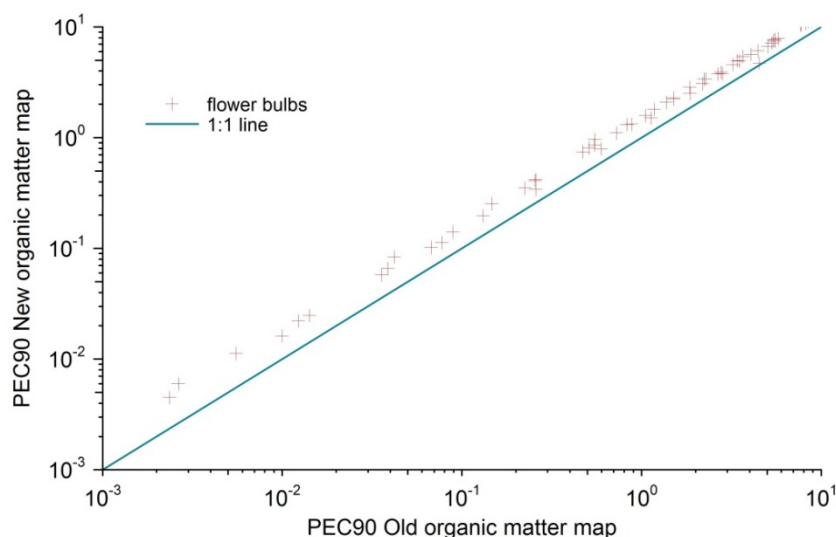
The calculations for the schematisation based on the 2017 soil organic matter map were done with PEARL model version 3.1.6 (20 January 2016). The SWAP version 2.0.9e of GeoPEARL version 3.3.3 has been replaced by the SWAP version 3.2.37. The spatial 90 percentile of the leaching concentrations for maize, cereals and flower bulbs were calculated with the old and the new schematisation. Calculations were done for a series of 120 substances covering a wide range of values of DegT50 (range 20 to 200 d) and  $K_{om}$  (range 0 to 250 L/kg). A listing of the DegT50-  $K_{om}$  combinations is given in Annex 1. The dosage was taken to be 1 kg/ha and the yearly application date was set to 26 May. The results of these calculations are presented in Figures 3.3 to 3.5. For cereals and flower bulbs the 90 percentile leaching concentration using the new schematisation is a factor 2 to 3 higher than using the old schematisation. For maize the difference increases to an order of magnitude for leaching concentrations below 0.1  $\mu\text{g/L}$ . For concentrations higher than 0.1  $\mu\text{g/L}$  the difference becomes smaller and the factor diminishes to a factor 2.



**Figure 3.3** The spatial 90 percentile leaching concentration ( $\mu\text{g L}^{-1}$ ) in the area of use for maize calculated on the basis of the 2004 and the 2017 organic matter map. Aggregation on a plot basis. Yearly application on 26 May. Activation energy 54  $\text{kJ mol}^{-1}$ .



**Figure 3.4** The spatial 90 percentile leaching concentration ( $\mu\text{g L}^{-1}$ ) in the area of use for cereals calculated on the basis of the 2004 and the 2017 organic matter map. Aggregation on a plot basis. Yearly application on 26 May. Activation energy  $54 \text{ kJ mol}^{-1}$ .



**Figure 3.5** The spatial 90 percentile leaching concentration ( $\mu\text{g L}^{-1}$ ) in the area of use for flower bulbs calculated on the basis of the 2004 and the 2017 organic matter map. Aggregation on a plot basis. Yearly application on 26 May. Activation energy  $54 \text{ kJ mol}^{-1}$ .

Due to the substantial differences in the target leaching concentration between the old and the new schematisation, the implications of the use of the new schematisation on the Dutch Decision Tree was investigated. The results of this investigation are described in Chapter 4.

### 3.3 Considerations on the parameterisation for GeoPEARL version 4.4.4

#### 3.3.1 Estimation of the organic-matter content in soils for fruit crops

The trend model is based on the division between either arable soil or grassland (via the coefficient  $\beta_3$ ). However, for some permanent crops (e.g. fruit crops), it is not clear in which category they fall. This section describes the decisions that were made for these crops and the underlying considerations.

Pome fruit (apples and pears) is by far the most important permanent crop (excluding permanent grassland). A fruit crop field in the Netherlands consists usually of a strip of bare soil ('zwarte grond') below the trees and a strip of permanent grass between the trees. The trees are usually 3 m apart; the bare soil strip is 1-1½ m wide and the grass strip is thus 1½-2 m wide. Most common is a bare soil strip of 1 m wide and a grass strip of 2 m wide (personal communication Van de Zande, 2017). The bare-soil strip is treated annually with a herbicide (by downward spraying) which keeps it free of weeds and grass during the growing season. In autumn and spring, there is commonly regrowth of weeds and grass on this strip.

The calculation procedure for the organic matter content in GeoPEARL assumes that fruit is an arable crop. The alternative would have been to assume that it is grassland. Organic matter contents of the top soil of permanent grass are typically two times higher than those of the top soil of annual crops (see e.g. Fig. 3 of Reijneveld et al., 2009, for Dutch data and Table 9.1 of Toth et al., 2013, for data at EU level). Pesticide applications via sideways and upward spraying in the fruit crops are directed towards the trees, thus also to the bare-soil strip below the trees. However, a considerable fraction of the dose is expected to be deposited on the grass strip between the trees. Thus a fruit field is essentially a two-dimensional system with respect to leaching with less leaching expected below the grass strip and more leaching expected below the bare-soil strip. Thus the question is whether the organic-matter parameterisation of GeoPEARL for the fruit crops is appropriate. It can be expected that the organic-matter content of the 2-m grass strip is likely to be underestimated. On the other hand it can be expected that the organic-matter content of the bare soil strip is somewhat lower than assumed in GeoPEARL because this bare soil strip receives less input of organic material than a soil grown with annual crops. To verify this, a review of the relevant available data is needed after having made a distinction between organic matter contents measured in the bare-soil strip of fields with fruit trees from those measured in the grass strip in these fields. An analysis by EFSA (2017) of the LUCAS dataset showed only comparative small differences between the frequency distributions of organic matter of (i) the annual crops and (ii) the permanent crops in the regulatory zone 'Centre'.

In the Netherlands, trees and small fruit crops like bushberries are grown without grass strips. Silviculture is a crop in GeoPEARL and the organic matter content in soils with this crop is estimated assuming that it is bare soil. The small fruit crops are not separately considered in GeoPEARL; they are part of the fruit crops area so also for these crops GeoPEARL assumes that they are arable.

EFSA (2017) assumes a non-uniform organic matter profile for the top 30 cm and differentiates between permanent crops with and without mechanical treatment as described in Table 3.2. However, this was based on only one measurement in citrus and one measurement in olives for the mechanical treatment (Beulke et al., 2015, p. 78). The non-uniform distribution of the organic matter in the top 30 cm is expected to have only a minor effect on the leaching. So in GeoPEARL a uniform organic matter content in the top 25-cm layer is assumed for fruit crops.

**Table 3.2** Multiplication factors for organic matter content for permanent crops with and without mechanical treatment as used by EFSA (2017).

Depth (cm)	Multiplication factor	
	with mechanical treatment	without mechanical treatment (continuous grass cover)
0-5	1.5	1.95
5-10	1.2	1.30
10-20	0.9	0.76
20-30	0.75	0.62

# 4 Calibration factors of the 2017 decision tree for leaching to groundwater

The preliminary calculations in Chapter 3 have shown the consequences for the leaching assessment using GeoPEARL with a schematisation based on the 2017 soil organic matter map. Therefore a systematic procedure was set up to find out what modifications are needed to ensure a consistency between the first and second tiers of the Dutch Decision Tree for leaching to groundwater. In the first tier, the Kremsmünster scenario is used and the 80 percentile of the leaching concentration is calculated by FOCUSPEARL. In tier 2 of the Decision Tree the 90<sup>th</sup> percentile leaching concentration in space is calculated by GeoPEARL in the area of use of the compound. This area of use is related to the area of the crop for which cultivation the compound is proposed to be used. This report is only valid for the decision tree using the current version of FOCUSPEARL.

## 4.1 Procedure for calculation of consistency between tiers

The substances for these computations were taken from Vanderborght et al. (2010). These substances cover a range of  $K_{om}$  and DegT50 combinations. The  $K_{om}$  and DegT50 values for these compounds are listed in Table 4.1. The Freundlich exponent of these substances was set at 0.9 and the molar activation energy for transformation was taken to be 65.4 kJ/mol.

**Table 4.1** Sorption coefficient and half-life for the test substances in VanderBorgh et al. (2010).

SubstanceId	$K_{om}$ (L/kg)	DegT50 (d)	SubstanceId	$K_{om}$ (L/kg)	DegT50 (d)
1	10	7	11	10	20
2	20	8	12	20	30
3	40	12	13	40	60
4	100	25	14	100	140
5	200	45	15	200	250
6	10	10	16	10	40
7	20	15	17	20	60
8	40	30	18	40	120
9	100	70	19	100	280
10	200	120	20	200	500

The application dates considered in the computations were the 15<sup>th</sup> of each month. Computations were done for all substance – application date combinations for all plots of the GeoPEARL schematisation, i.e. 6405 and selection the GeoPEARL crop 'TotalAgriculturalArea'. In an assessment for tier 2 the default number of plots is 250. For each GeoPEARL crop a different set of plots is selected. For the selection of plots in the new GeoPEARL version, the option 'Neighbour' was used. As computations for each substance – application were done for all plots, a post processing procedure was developed to select the output of the 250 plots for each GeoPEARL crop. Although the ploughing dates for the crop type 'TotalAgriculturalArea' are the same as for most GeoPEARL crops, for some crops there can be differences. For TreeNursery, FruitCulture and Silviculture no ploughing occurs, so the procedure adopted would result in an overestimation of the target leaching concentration for these crops. Because the number of crops associated with the Kremsmünster scenario is smaller than the number of crops in GeoPEARL, the crop list table as used in the Dutch registration procedure has been used. In Table 4.2 the equivalent crop in the Kremsmünster scenario is listed for each GeoPEARL crop.

In this way the 90<sup>th</sup> percentile leaching concentration in space for each crop – substance – application date combination using the new GeoPEARL version was compared with the 80 percentile of the leaching concentration as calculated for the corresponding crop – substance – application date

combination by FOCUSPEARL for the Kremsmünster scenario. The total number of these combinations is 5760. However, not all application times are realistic for all crops. Based on expert judgment the relevant application season was specified for all GeoPEARL crops. The relevant periods are listed in Table 4.3. When taking only the relevant application – crop combinations into account the total number of combinations for the comparison was 4920.

**Table 4.2** *Ctgb crop list in the Decision Tree for leaching to ground water.*

	GeoPEARL crop	FOCUS Kremsmuenster crop
1	Potatoes	Potatoes
2	Strawberries	Strawberries
3	Asparagus	Potatoes
4	SugarBeets	Sugarbeets
5	LeafVegetables	Cabbage
6	plants_for_commercial_purposes	Winter Cereals
7	Floriculture	Winter Cereals
8	FlowerBulbs	Winter Cereals
9	TreeNursery	Winter Cereals
10	Fallow	NoCrop
11	FruitCulture	Apples
12	Cereals	Winter cereals
13	Grass	Grass
14	GrassSeed	Grass
15	GreenManuring	Winter Oil Seed Rape
16	Vegetables	Carrots
17	Cannabis	Winter Cereals
18	Silviculture	Winter Cereals
19	Cabbage	Cabbage
20	Maize	Maize
21	RemainingAgriculturalCrops	Winter Cereals
22	Legumes	Beans
23	Leek	Onions
24	Onions	Onions

**Table 4.3** *Specification of the application season for the GeoPEARL crops.*

Crop	Application season
Potatoes	March - November
Strawberries	March - November
Asparagus	March - October
SugarBeets	March - November
LeafVegetables	January - December
plants_for_commercial_purposes	March - October
Floriculture	January - December
FlowerBulbs	January - December
TreeNursery	January - December
Fallow	March - November
FruitCulture	January - December
Cereals	January - December
Grass	March - November
GrassSeed	March - November
GreenManuring	January - December
Vegetables	January - December
Cannabis	April - September
Silviculture	January - December
Cabbage	January - December
Maize	April - October
RemainingAgriculturalCrops	January - December
Legumes	March - October
Leek	January - December
Onions	January - December

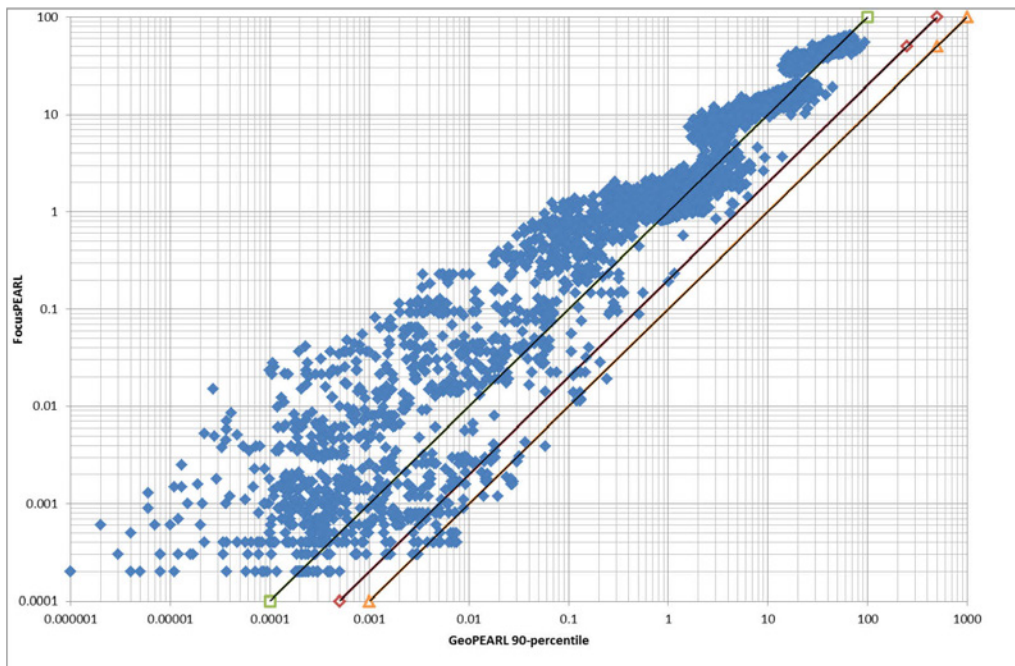
It should be noted that the organic matter content in the topsoil of arable soils is different from the content in grassland soils. For the GeoPEARL computations with the new version the organic matter content for the top soil in arable soils was selected. This is correct for all GeoPEARL crops, except grass. The organic matter in the topsoil in the plots selected for grass are based on the content in this layer for arable land use. Because organic matter contents in the topsoil in grasslands are higher than that in arable land, the leaching concentrations calculated for the GeoPEARL crop 'grass' using the post processing procedure is likely to overestimate the leaching to groundwater in grasslands.

The GeoPEARL calculations using a schematisation based on the 2017 soil organic matter map were done with PEARL model version 3.1.6 (20 January 2016) in combination with SWAP version 3.2.37. The assessments were executed on the computation grid of Alterra.

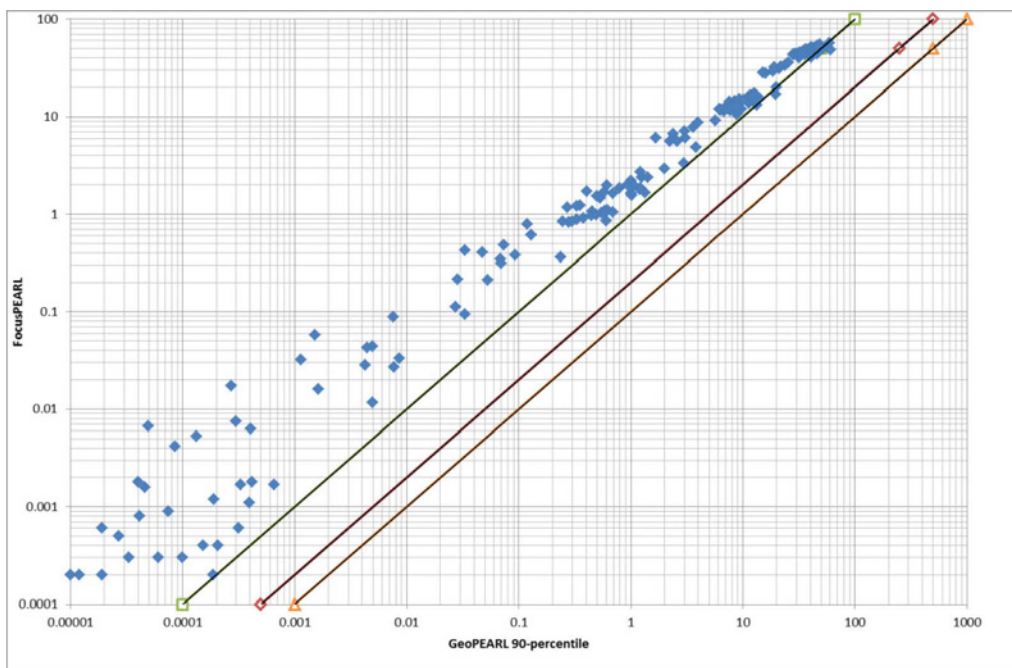
## 4.2 Results of calculations and effect of calibration factor

The results for all crops excepting grass are presented in Figure 4.1 and those for grass are presented in Figure 4.2. The results in Figure 4.1 show that for arable crops many results are below the 1:1 line. This means that the PEC90 calculated using GeoPEARL in tier 2 is higher than the PEC80 calculated using FOCUSPEARL in tier 1. The results shown for grass in Figure 4.2 do not show the same distribution. For grass the results for tier 1 are more conservative than for tier 2. The differences can be expected to even greater, because the organic matter contents in the topsoil were taken from the soil organic matter predictions for arable land.

The inconsistency between the first and second tiers could be remedied by the introduction of a calibration factor. The tier-1 calibration factor is defined as the factor with which the FOCUS leaching concentration from the FOCUS Kremsmünster scenario for crop  $x$  (as calculated in tier 1) has to be multiplied to ensure that the endpoint of tier 1 is more conservative than a GeoPEARL calculation for this crop  $x$ . The use of this factor would result in higher values for the leaching concentrations as calculated by FOCUSPEARL for tier 1. In Figure 4.1 the effect of calibration factors 5 and 10 are shown. When using a factor 5, the outcome of the GeoPEARL calculation is higher than that of the FOCUS calculation for a large number ( $N=83$ ) of crop – application – substance combinations. This number  $N$  decreases to 34 when using a calibration factor of 10.



**Figure 4.1** PEC80 FOCUSPEARL vs PEC90 GeoPEARL. All GeoPEARL crops, excepting Grass. All relevant application time – crop combinations. Calibration factor 1 (line with green squares), 5 (line with red diamonds) and 10 (line with orange triangles).



**Figure 4.2** PEC80 FOCUSPEARL vs PEC90 GeoPEARL. Grass only. Application season March - November. Calibration factor 1 (line with green squares), 5 (line with red diamonds) and 10 (line with orange triangles).

As the leaching to groundwater for autumn/winter applications is higher than for spring/summer applications, a more detailed comparison was made for applications in the period from March to August and for applications in the period from September to February. The results of the comparison for the applications in the period from March to August in combination with a calibration factor 5 is given in Figure 4.3. The comparison is focused on the concentration range of 0.01 to 1  $\mu\text{g L}^{-1}$ . For this range, there is only one crop - substance - application time (csa) combination that results in a higher tier 2 result than the tier 1 result, i.e. for an application of substance 2 in flower bulbs in August.

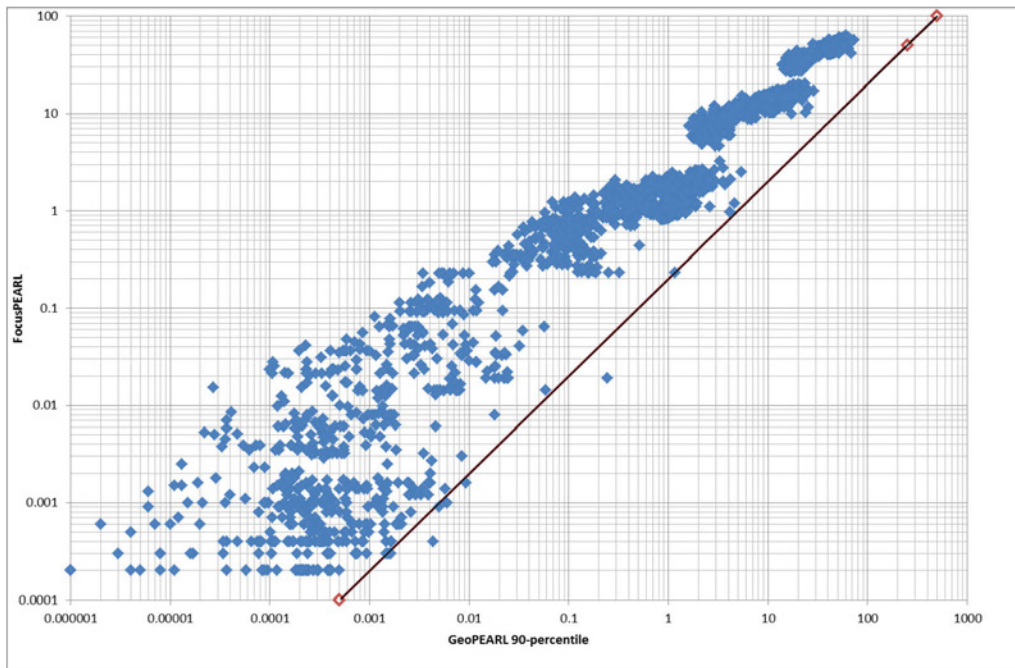
The results of the comparison for the applications in the period from September to February in combination with a calibration factor 5 is given in Figure 4.4. In the concentration range of interest there are 39 csa combinations (from a total of 4920) that result in a higher tier 2 result than the tier 1 result. The applications are mostly in October (13) and November (25). The substances associated with these points are substances 2 (once), 3 (11 cases), 4 (25 cases) and 5 (two cases). When introducing a calibration factor of 10, the number of non-consistent points reduces from 39 to 17. The results for the effect of this factor is shown in Figure 4.4. These points are associated with substances 3 (4 cases), 4 (11 cases), and 5 (2 cases). The crops in these cases are fruit (3 cases), grass seed (2 cases), vegetables (one case), leafy vegetables (2 cases), potatoes (2 cases), cabbage (2 cases), and one case each for legumes, cereals, onions, sugar beet and remaining crops. Interestingly, the substances in the non-consistent cases have a ratio of  $K_{om}$  to DegT50 of about 4. The  $K_{om}$ -DegT50 diagram for all substances is shown in Figure 4.5. In Figure 4.6 the substances are shown with DegT50 values of up to 100 d. In this Figure the number of substances with a ratio of the  $K_{om}$ -DegT50 between 3.5 and 4.5 is shown more clearly (16 out of total number of 365 substances).

On the basis of these results a calibration factor of 5 would be enough to ensure consistency between tier 1 and tier 2 for applications in the period from March to August. A higher calibration factor is needed to ensure consistency between tier 1 and tier 2 for applications in the period of September to February. For most crop - substance - application time combinations a calibration factor of 10 would be enough. For 17 out of 4920 combinations (0.4% of the cases assessed) the results of tier 2 would be higher than the results of tier 1.

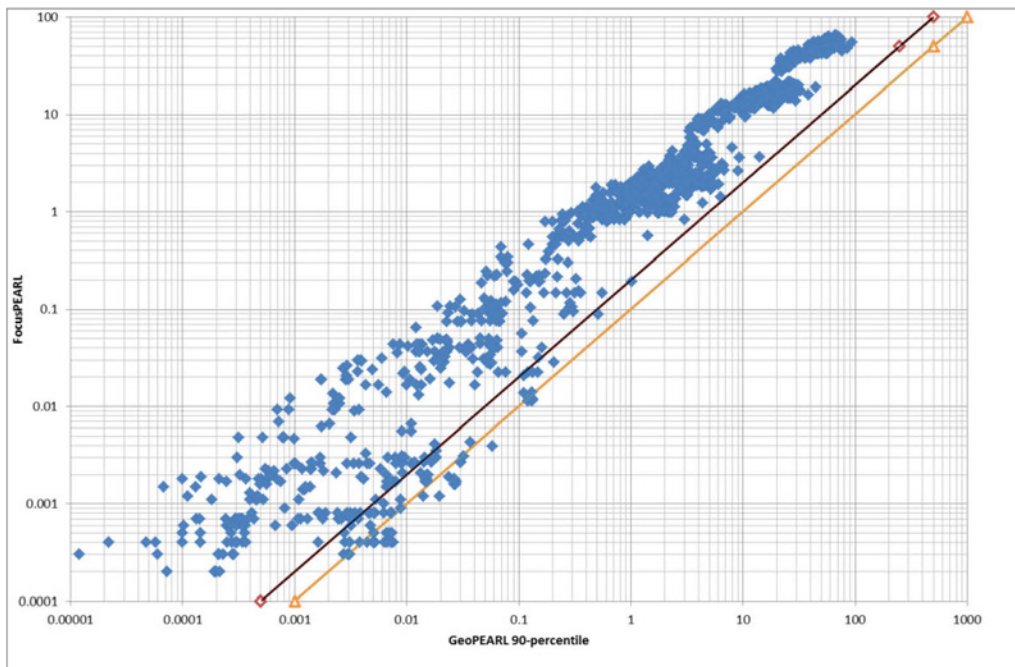
There could be an additional criterion to ensure consistency for all crop - substance combinations for applications in the period of September to February. As mentioned above, most substances in the



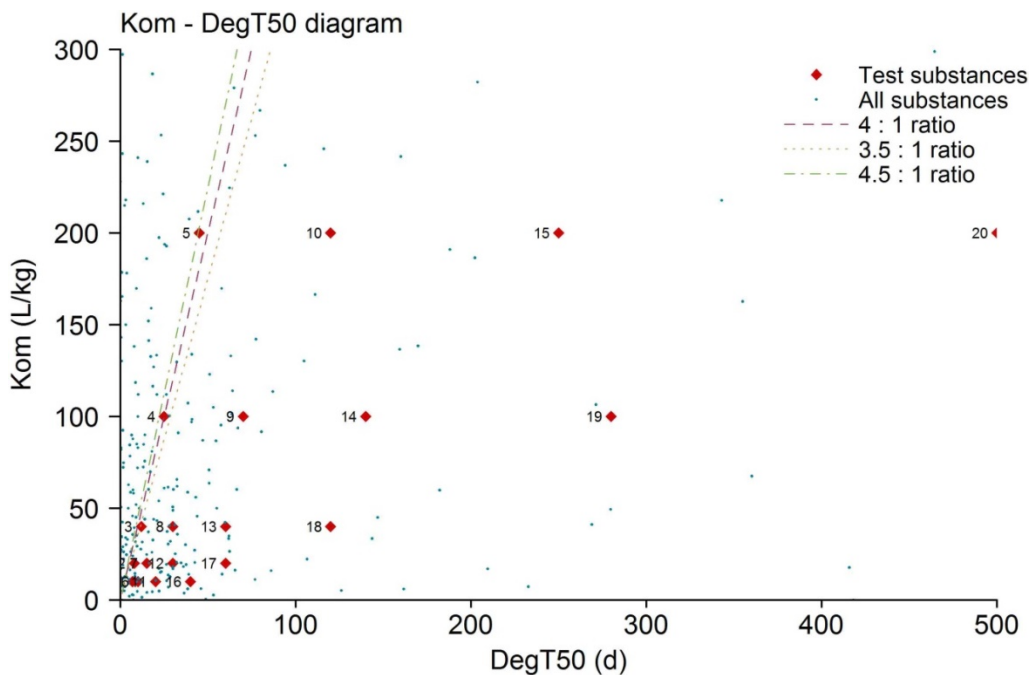
non-consistent cases have a ratio  $r$  of  $K_{om}$  to DegT50 of about 4. So it could be an option to skip tier 1 calculations for compounds with  $r < 4.5$  and  $r > 3.5$  and that tier 2 GeoPEARL assessments need to be done straightaway.



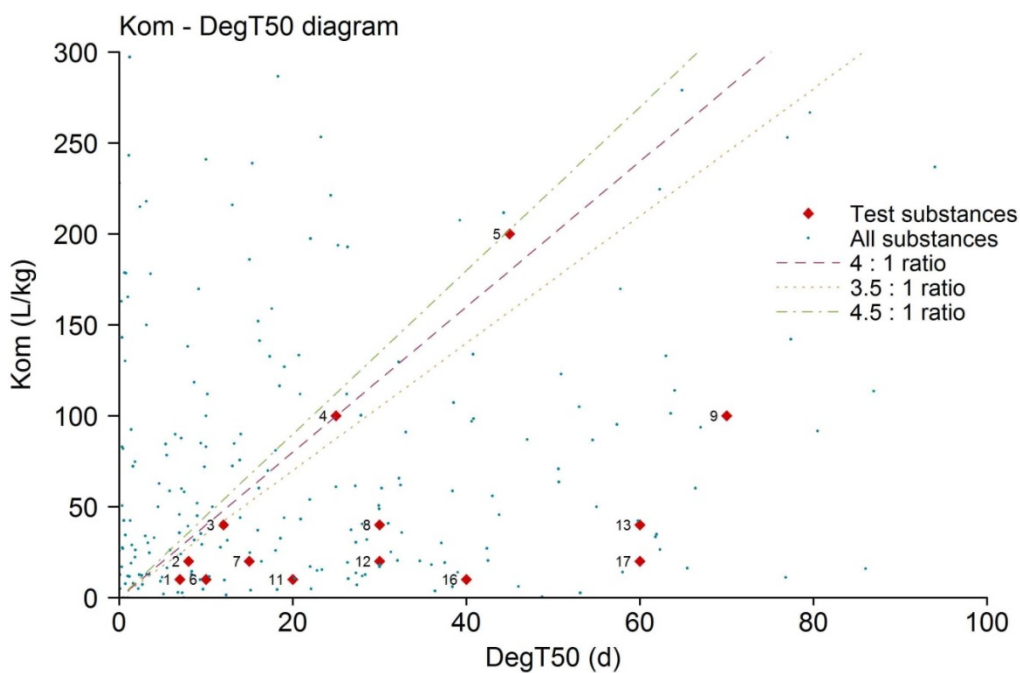
**Figure 4.3** PEC80 FOCUSPEARL vs PEC 90 GeoPEARL for all GeoPEARL crops, excepting grass. All relevant application time – crop combinations. Calibration factor 5 (line with red diamonds). Applications from March to August.



**Figure 4.4** PEC80 FOCUSPEARL vs PEC 90 GeoPEARL for all GeoPEARL crops, excepting grass. All relevant application time – crop combinations. Calibration factor 5 (line with red diamonds) and 10 (line with orange triangles). Applications from September to February.



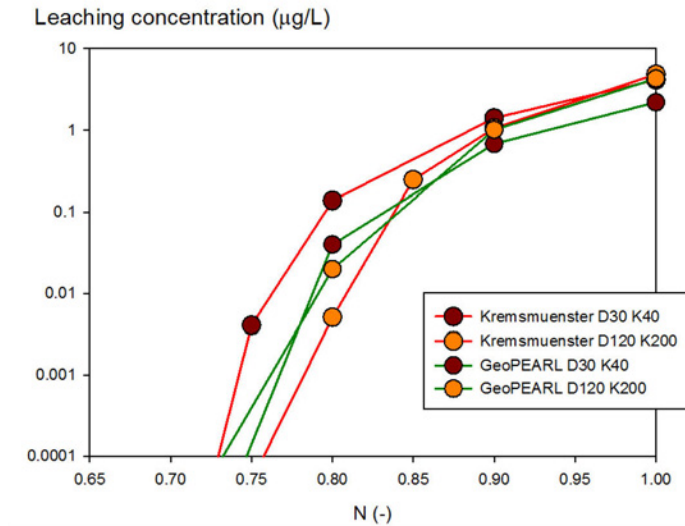
**Figure 4.5**  $K_{om}$ -  $DegT50$  diagram for the 20 test substances. Lines indicate a ratio of 3.5, 4 or 4.5 between the  $K_{om}$  and the  $DegT50$  value. Dots represent active substances or metabolites of active substances registered in the Netherlands (Dorgelo, 2006).



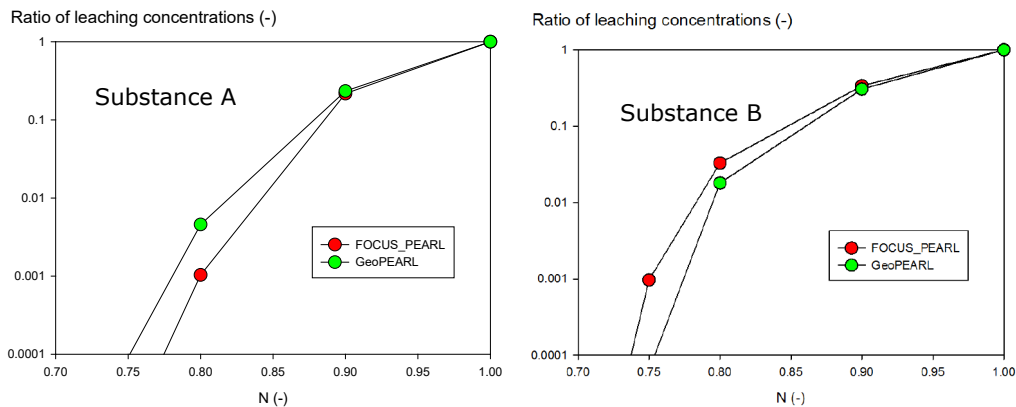
**Figure 4.6**  $K_{om}$ -  $DegT50$  diagram for the test substances with  $DegT50$  values up to 100 d. Lines indicate a ratio of 3.5, 4 or 4.5 between the  $K_{om}$  and the  $DegT50$  value. Dots represent active substances or metabolites of active substances registered in the Netherlands (Dorgelo, 2006).

The comparison between FOCUS Kremsmünster and GeoPEARL in the above figures was based on a Freundlich exponent  $N$  of 0.9. In dossiers,  $N$  ranges usually between 0.8 and 1.0. Therefore the effect of  $N$  was checked for two substances ( $DegT50 = 30$  d and  $K_{om} = 40$  L/kg and  $DegT50 = 120$  d and  $K_{om} = 200$  L/kg). Results in Figure 4.7 show that both FOCUS Kremsmünster and GeoPEARL are very sensitive to  $N$  and that this sensitivity is about equal.

Figure 4.8 shows the same results but now scaled to unity for  $N = 1$ . Results for  $DegT50 = 30$  d and  $K_{om} = 40$  L/kg show that FOCUS Kremsmünster generates a smaller decrease on a relative scale than GeoPEARL when  $N$  decreases from 0.9 to 0.8 and results for  $DegT50 = 120$  d and  $K_{om} = 200$  L/kg show the opposite. This indicates that the calibration factor developed above is conservative enough for a substance with a  $DegT50$  of 30 d and a  $K_{om}$  of 40 L/kg but that it may not be conservative enough for a substance with a  $DegT50$  of 120 d and a  $K_{om}$  of 200 L/kg. So there is in general no guarantee that the calibration factor developed above works also well for  $N$  values around 0.8. We propose therefore that the above procedure is repeated for  $N = 0.8$  to check this.



**Figure 4.7** Leaching concentrations calculated using FOCUSPEARL and GeoPEARL for substances with different values for  $N$ .



**Figure 4.8** Ratio of leaching concentrations calculated using FOCUSPEARL and GeoPEARL for substances with different values for  $N$ . Ratio equal to 1 when  $N$  equal to 1. Substance A:  $DegT50$  120 d,  $K_{om}$  200 L/kg; Substance B:  $DegT50$  30 d,  $K_{om}$  40 L/kg.

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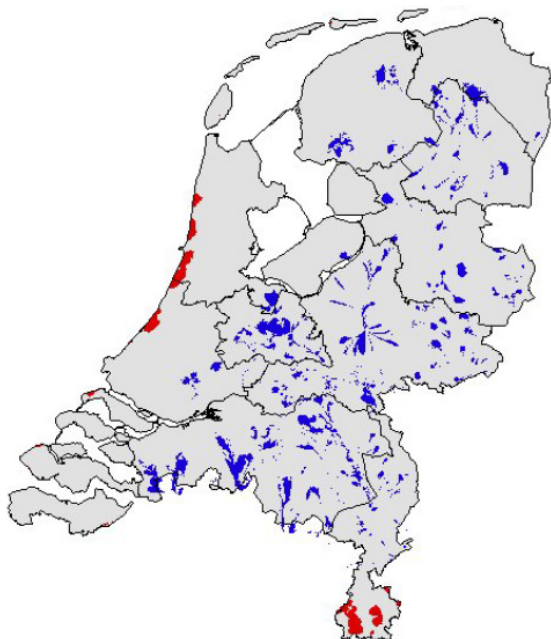
# 5 Organic matter in groundwater abstraction areas

The general aim of the Dutch pesticide registration procedure is to protect the groundwater as a source of drinking water. In an earlier study (Kruijne et al., 2004) it was found that ground water abstraction areas are up to five times more vulnerable to leaching of pesticides than the groundwater in the Dutch agricultural area as a whole. This was mainly because organic matter in groundwater abstraction areas was lower than organic matter in the Dutch agricultural area as a whole. In this paragraph, we will assess whether this also holds for the 2017 soil organic matter map.

## 5.1 Groundwater abstraction areas

The map with the ground water abstraction areas used for this analysis (see Figure 5.1) is the same as the map used by Kruijne et al. (2004). This map is composed of two sources. For most drinking water production wells, the abstraction areas were obtained in separate studies with the saturated groundwater model LGM (Kovar et al., 1992; 1998). The size and shape of these areas result from the calculated streamlines in the saturated groundwater. Within the boundaries of these areas, water percolating into the saturated zone will finally reach the drinking water production well, no matter how long the travel time may be.

In the coastal regions and in the most southern part of the Netherlands the streamlines around the drinking water production wells were not calculated yet. In these regions, groundwater protection areas were selected instead of groundwater abstraction areas. The boundaries of these areas may result from calculated travel times of the saturated groundwater towards the well (e.g. 25 years), but the shape of these areas is also based on local topography. As a result of this, especially in the most southern part of the Netherlands these areas will not fully coincide with the true abstraction areas.



**Figure 5.1** Groundwater abstraction areas used by Kruijne et al. (2004).

It should be noted that the map of ground water abstraction areas used by Kruijne et al. (2004) is based on the situation in the 1990s, which is almost 25 years ago. Because of problems with nitrate contamination, some ground water abstraction wells have been closed and others are now in deeper aquifers. This may affect the organic matter distribution in groundwater abstraction areas. KWR Watercycle Research Institute made a more recent inventory of groundwater abstraction wells (Leunk, 2012). It is advised to use this information to create a new map of groundwater abstraction areas. This should preferably be done with the Netherlands Hydrological Instrument (De Lange et al., 2014), because this is the commonly agreed model for integrated water management in the Netherlands.

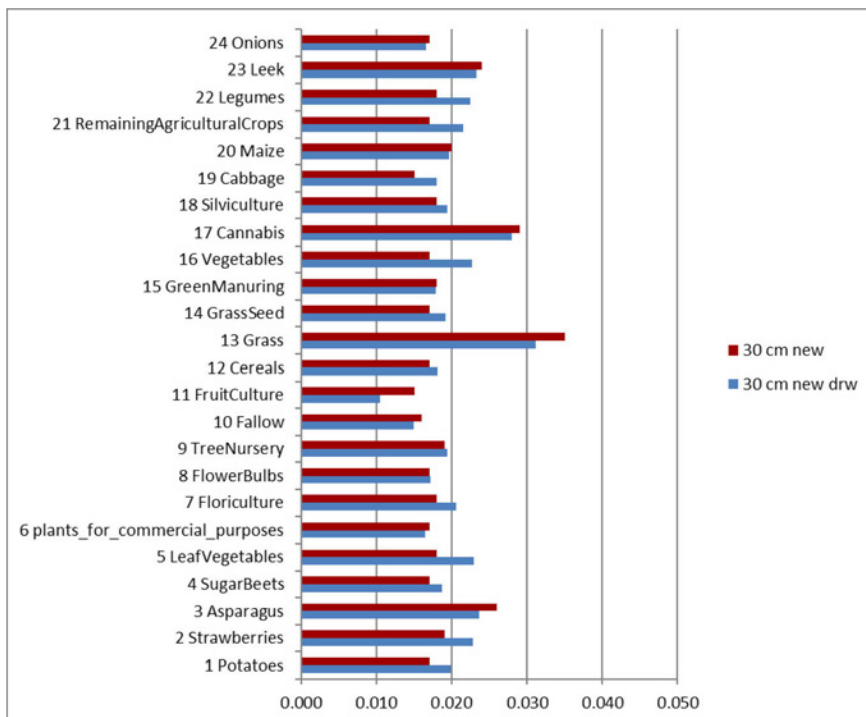
## 5.2 Organic matter in groundwater abstraction areas

Organic matter is the most important spatially-distributed soil parameter affecting pesticide leaching (Van den Berg et al., 2009; Heuvelink et al., 2010). It is therefore relevant to compare organic matter distribution in groundwater abstraction areas and in the Dutch agricultural area as a whole. This comparison was done for all GeoPEARL crops; results are shown in Figure 5.2 (for the top 30 cm) and 5.3 (for the top 100 cm). These figures show that the difference in organic matter content between groundwater abstraction areas and the Netherlands as a whole is generally small (maximum differences generally less than 10%). For many crops, organic matter contents are even higher in groundwater abstraction areas. Only in the case of silviculture and plants grown for commercial purposes, organic matter content in groundwater abstraction areas is significantly lower than organic matter in the Netherlands as a whole. These crops, however, comprise only a small area (silviculture 670 ha and plants for commercial purposes 30 ha).

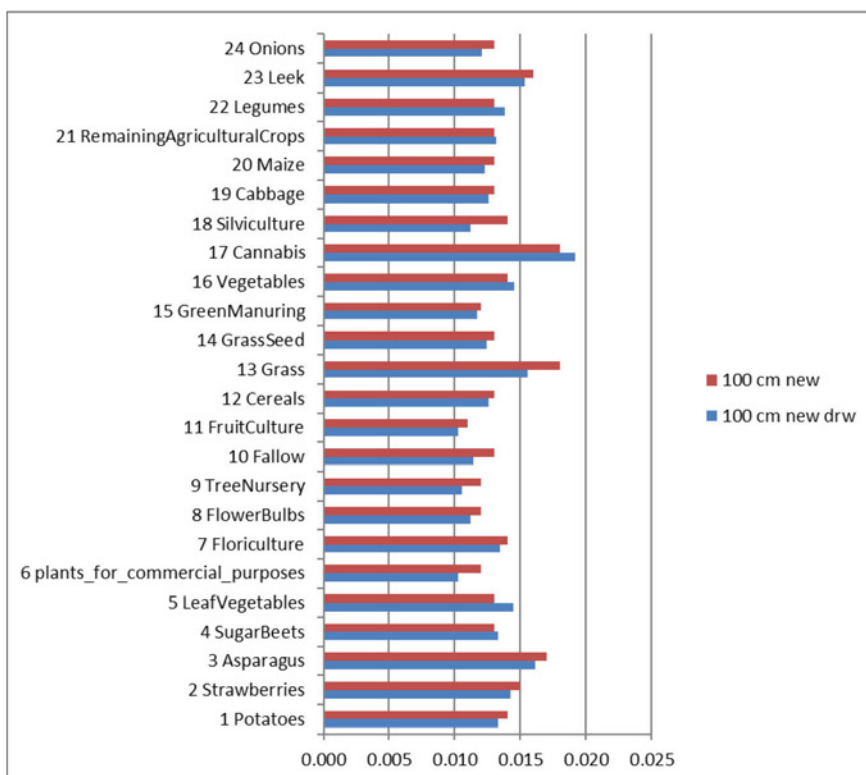
Kruijne et al. (2004) also compared the organic matter content of soil in groundwater abstraction areas with organic matter content in the Netherlands as a whole. They directed this analysis towards the five most important crops, i.e. grass, maize, cereals, potatoes and sugar beets. These crops together cover 90% of the Dutch agricultural area and 92% of the area of groundwater abstraction regions. Table 5.1 shows that differences between groundwater abstraction area and the total agricultural area are slightly less for GeoPEARL 4.4.4 than for Kruijne et al. (2004). It should be noted, however, that differences reported by Kruijne et al. (2004) were already small.

**Table 5.1** The spatial 10th percentile of soil organic matter (0-1 m below soil surface) within ground water abstraction areas and in the total Dutch agricultural area.

	Kruijne et al. 2004		GeoPEARL 4.4.4	
	Groundwater abstraction area	Total agricultural area	Groundwater abstraction areas	Total agricultural area
Grass	0.017	0.020	0.016	0.018
Maize	0.017	0.018	0.012	0.013
Cereals	0.011	0.014	0.013	0.013
Potatoes	0.016	0.015	0.013	0.014
Sugar beets	0.011	0.014	0.013	0.013
All crops (n=24)	0.016	0.018	0.013	0.013



**Figure 5.2** 10-percentiles of organic matter content of the top 30 cm of the soil in groundwater abstraction areas compared with the organic matter content for the Dutch agricultural area as a whole.



**Figure 5.3** 10-percentiles of organic matter content of the top 100 cm of the soil in groundwater abstraction areas compared with the organic matter content for the Dutch agricultural area as a whole.

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## 5.3 Consequences for the leaching concentration

The above exercise shows that differences between the organic matter content of groundwater abstraction areas and the Dutch agricultural area as a whole are smaller for GeoPEARL 4.4.4 than for earlier model versions. Given that all other model parameters were kept equal, it is to be expected that differences are also less for the leaching concentration. This makes it questionable whether the factor of 10 that is currently used to protect groundwater abstraction areas (Chapter 6) is always necessary. It should be noted, however, that organic matter is not the only factor determining the vulnerability of groundwater abstraction areas. Other factors such as the permeability of the soil and the regional hydrological situation may be important as well. The vulnerability of the groundwater abstraction areas can therefore not *a priori* be determined. For this reason, it is advised to reassess the vulnerability of the groundwater abstraction areas using the methodology described in Kruijne et al. (2004).

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# 6 The proposed 2017 decision tree for leaching to ground water

In the previous chapters the development of the 2017 organic matter map (Chapter 2) and its implementation in GeoPEARL version 4.4.4 (Chapter 3) are presented. The introduction of GeoPEARL version 4.4.4 with the 2017 organic matter map in tier 2 of the Dutch decision tree on leaching to groundwater, requires a check on the consistency of the tiers. In Chapter 4 the consistency between the first and the second tier was investigated and calibration factors are proposed. The need for a safety factor on the calculated leaching concentration in tier-1 and tier-2, in order to protect groundwater abstraction areas, was investigated in Chapter 5. Based on this information, a proposal for the 2017 decision tree is described in this chapter.

## 6.1 The Dutch national protection goal for leaching to groundwater

In this section, the national protection goal for leaching to groundwater is inferred from current legislation. In the Netherlands, approximately 60% of drinking water is abstracted from groundwater. The need to protect this source is described in general terms in the Groundwater Directive of the European Union: "Groundwater in bodies of water used for the abstraction of drinking water or intended for such future use must be protected in such a way that deterioration in the quality of such bodies of water is avoided in order to reduce the level of purification treatment required in the production of drinking water." The ambition to protect both groundwater abstraction areas and possible future sources is also included in the Dutch Water act and recently recalled in the "Structuurvisie voor de Ondergrond (STRONG)".

The above-mentioned protection goal for groundwater gives only a very general ambition to protect groundwater. It does not describe explicitly how much groundwater needs to be protected, when it should be protection and at what level. A protection goal can only form the basis for a decision tree when it is worked-out in quantitative terms. Such a worked-out protection goal is called a specific protection goal and should be the same for all tiers in a decision tree. A specific protection goal should define the following elements (e.g. EFSA, 2012; Anonymous, 2015):

- (i) The type of concentration (e.g. concentration in the top m of groundwater);
- (ii) The temporal dimension of this concentration (e.g. annual average concentration);
- (iii) The spatial unit (e.g. agricultural field);
- (iv) The spatial population of spatial units (e.g. only fields without brackish groundwater);
- (v) The multi-year temporal population of concentrations (e.g. years in the repetition sequence);
- (vi) The combination of spatio-temporal percentile to be taken from the spatio-temporal population of concentrations (e.g. 90-50 percentiles).

The Dutch specific protection goal for leaching to groundwater is described in article 8e of the 'Besluit gewasbeschermingsmiddelen en biociden'. This article focusses on the details of the registration procedure without giving a description of the general protection goal. More details are described in Van der Linden et al. (2004; RIVM report 601450019) to which is referred in article 8e. From article 8e and RIVM report 601450019 the following specification of the protection goal can (implicitly) be derived:

- (i) the type of concentration is the resident concentration in groundwater at 10 m below the soil surface;
- (ii) The temporal dimension is the yearly average concentration;
- (iii) The spatial unit is a treated field (this is, however, not completely clear from this article);
- (iv) There are two protection goals with different spatial populations of the spatial units: one consists of all treated fields in the Netherlands and one consists of the treated fields in the groundwater protection areas;



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- (v) The multi-year temporal population of concentrations consists of a time series of the annual average concentrations as defined in item (ii);
- (vi) the 90<sup>th</sup> spatial percentile of the median in time is taken. The endpoint is 0.1 µg/L for both protection goals.

With respect to the interpretation of results of monitoring studies, article 8e does not provide guidance. However, Cornelese et al. (2003) provided guidance on handling of monitoring studies and wrote that the null hypothesis to be tested is whether the 90<sup>th</sup>-percentile in space of the long-term average concentration in groundwater at 10 m depth is above 0.1 µg L<sup>-1</sup> (their p. 13). This is consistent with item (vi) of the protection goal as described above.

From the above, it is obvious that the market share of the pesticide is not considered relevant for the protection goal: GeoPEARL simulations are run for the whole area of the crop considered and this simulation is expected to be representative of the spatial population of fields treated with this pesticide (whereas the market share is never higher than about 40% in the Netherlands; Adriaanse et al., 2008).

For the interpretation of monitoring results, it is relevant to note that the groundwater sampled at 10 m depth may originate from water that has infiltrated into the soil at some distance from the sampling site. Uffink and Van der Linden (1998) showed that groundwater at 10 m depth in infiltration areas can vary significantly in age and still has preserved much of the variability in concentrations that occurred in the top layer of the groundwater. The infiltration pattern in space and time can still be recognised at the depth of 10 m. Diffusion and dispersion in the groundwater occurs, but the effect is still limited at the depth of 10 m.

## 6.2 The current decision tree for leaching

In 2004 a new decision tree for the assessment of the risk for leaching to groundwater was developed, in which also the GeoPEARL model was introduced (Van der Linden et al. 2004). The main reason for the development of the new decision tree was the need to harmonise the national authorisation of plant protection products (PPP) with the European procedure for approval of active substances. In addition, the availability of spatially distributed data and the GeoPEARL model, made it possible to explicitly test the vulnerability objectives of the decision tree. The new decision tree came into force in January 2005, and is included in the Dutch evaluation manual from April 2006 (Cornelese and Pol, 2006).

The 2004 decision tree follows a tiered approach in which earlier tiers are more stringent than later tiers, but require less information and effort from the applicant who seeks registration of a PPP. For all tiers the same leaching criterion is used:

*The concentration in groundwater at 10 m depth should be less or equal to 0.1 µg L<sup>-1</sup> under at least 90% of the potential area of application for at least 50% of the time*

In the first tier, the 80<sup>th</sup> percentile in time of the annual average leaching concentration at a target depth of 1 m (PEC80<sup>2</sup>) is obtained with FOCUS PEARL for the FOCUS Kremsmünster scenario, according to the European groundwater assessment procedure for approval of active substances (Anonymous, 2014). The potential area of use is not taken into account in the first tier. The second tier involves calculations with GeoPEARL, which calculates the 90<sup>th</sup> areal percentile of the median leaching concentration at a target depth of 1 m under the potential area of use (PEC90). In a separate study it was investigated whether an assessment for the total potential area of use sufficiently protects the groundwater in groundwater protection areas (Kruijne et al., 2004). It was concluded that the PEC90 for groundwater protection areas as a whole can be up to five times higher than those for

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<sup>2</sup> In the European procedure a scenario with an 80th percentile sensitive soil and an 80th percentile value for weather is used. The resulting 80<sup>th</sup> percentile in time of the annual average leaching concentration than approximates the overall 90th percentile concentration considering the vulnerability associated with both soil and weather.

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the total potential area of use. Therefore, a safety factor of 10 was introduced for groundwater protection areas where the calculated leaching concentration at the target depth of 1 m, in either a tier 1 calculation using FOCUS PEARL or a tier 2 calculation using GeoPEARL, must be  $<0.01 \mu\text{g L}^{-1}$ . In cases where the predicted leaching concentration is  $> 0.01 \mu\text{g L}^{-1}$  but  $\leq 0.1 \mu\text{g L}^{-1}$  it should be indicated on the label of the product that application in groundwater protection areas is prohibited..

### 6.3 The proposed 2017 decision tree for leaching

The revision of the soil organic matter map has led to an inconsistency in the tiered approach of the decision tree. Especially for autumn applications the GeoPEARL version based on the 2017 soil organic matter map calculates higher concentration than FOCUS PEARL for the Kremsmünster scenario. In Chapter 4 results of calculations have been presented for 20 example substances for all GeoPEARL crops and twelve different application timings (i.e. 15<sup>th</sup> day of every month). The results of this comparison have been used to derive the value for the calibration factor for the results of the first tier to maintain consistency between the first and the second tier. For spring applications (March 1 – August 31), a calibration factor of 5 is necessary to ensure consistency between these tiers. For autumn applications (September 1 – February 29), a calibration factor of 10 for is necessary to maintain a consistent decision tree for most substances.

On the basis of the results of the calculations presented in this report, it is no longer necessary to make an exception for flower bulbs as described in the Dutch evaluation manual (i.e. tier 2 calculation required if tier 1 result is not  $<< 0.01 \mu\text{g L}^{-1}$ ). Neither is it necessary to skip tier 1 for compounds with a  $K_{om}$  of less than  $10 \text{ L kg}^{-1}$  and a  $DegT50$  of less than 10 d as in the 2004 Decision Tree.

There could be an additional criterion to ensure consistency for all crop – substance combinations for applications in the period of September to February. As mentioned in section 4.2, most substances in the non-consistent cases have a ratio  $r$  of  $K_{om}$  to  $DegT50$  of about 4. So full consistency could be maintained by introducing a criterion on this ratio. For compounds with  $r < 4.5$  and  $r > 3.5$  tier 1 calculations could be skipped, so for these compounds tier 2 GeoPEARL assessments need to be done straightaway.

In Chapter 5 it was checked whether the safety factor of 10 for use in groundwater protection areas was still necessary. A comparison was made between the 10<sup>th</sup>-percentile of organic matter in groundwater abstraction areas and in the Dutch agricultural area as a whole for all GeoPEARL crops based on the 2017 organic matter map. This showed that depending on the crop the organic matter content in groundwater abstraction areas can be either lower or higher than in the Dutch agricultural area as a whole. This implies that depending on the crop, the 90<sup>th</sup>-percentile of the leaching concentration in groundwater abstraction areas can be either higher or lower than the concentration in the Dutch agricultural area as a whole. However, in order to make a well substantiated proposal regarding the safety factor for use in groundwater protection areas, a comparison based on predicted leaching concentration is required as was done in the study by Kruijne et al. (2004).

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# 7 Conclusions and recommendations

## 7.1 Conclusions

A methodology was developed to prepare separate organic matter maps for grassland and arable fields using digital soil mapping techniques. This distinction had not been made during the development of the organic matter map for GeoPEARL that has been used to date. The mapping consisted of two steps. First, a trend model was calibrated using the mapped soil type and land-use (arable or grassland) as a predictor. This step used the data from the Dutch Soil Sampling Scheme, which consisted of samples from 1210 locations that were selected using a well-defined stratified random sampling scheme. The next step consisted of a 3D-geostatistical interpolation procedure of the residuals using about 770 000 observations of soil organic matter. The advantage of this procedure is that regional differences within mapping units are accounted for.

The new soil organic matter maps were compared to the independent Reijneveld dataset, which is based on some 2 million samples from agricultural fields. This comparison revealed that the agreement between the 2017 soil organic matter map and the measurements is generally good except for peat areas. The difference for the peaty soils can be partly explained by the fact that the Reijneveld samples have been collected in the period 1994 – 2004, so the effect of peat oxidation since then is not taken into account in the comparison.

The accuracy of the 2017 soil organic matter map was quantified by the variance of the prediction error. The results of this analysis showed that the accuracy of the 2017 soil organic matter map is highest in areas where many observation points are available (e.g. in the East and South of the Netherlands) and less in areas with fewer observation points (e.g. West and reclaimed land in Centre). The most effective manner to improve the overall quality of the map is by doing more measurements on organic matter in areas with comparatively few observation points. These points could then be included in the dataset needed for the interpolation step of the procedure to create the new organic matter map.

As expected, organic matter contents in soils according to the 2017 soil organic matter map are lower than those according to the soil organic matter map that has been used in GeoPEARL so far. GeoPEARL simulations for 20 substances with different  $K_{om}$  and  $DegT50$  values showed that the 90<sup>th</sup>-percentile concentration increased by a factor of 2-10 depending on the crop type. This led to an inconsistency in the tiered approach of the Dutch Decision Tree for leaching to groundwater. Especially for autumn applications the GeoPEARL version based on the 2017 soil organic matter map calculates higher target leaching concentrations at 1 m depth than FOCUS PEARL for the Kremsmünster scenario. Simulations for the example substances showed that a calibration factor of 5 is necessary to ensure consistency between these tiers. For autumn applications, a calibration factor of 10 for is necessary to maintain a consistent decision tree for most substances.

## 7.2 Recommendations

### 7.2.1 Improving model performance for smaller areas including groundwater abstraction areas

The current schematisation of GeoPEARL consists of 6 405 fixed unique combinations of soil type, drainage system, climate district and land-use type (so-called plots). This leads to uncertainty of the model predictions for smaller areas, e.g. for individual groundwater abstraction areas and for less common crops like asparagus and onions. The reason is that the uncertainty in the predicted organic matter content is larger for small areas than for larger areas like the crop areas for maize and cereals,

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as they do not overlap completely with these fixed unique combinations. To improve the reliability of model predictions for these smaller areas, a more flexible schematisation procedure that allows for the derivation of unique combinations that overlap entirely with the areas of interest would be needed. With the currently used STONE schematisation, this is not possible. We therefore recommend to link with current efforts to develop a revised STONE schematisation based using NHI, the Netherlands Hydrological Instrument, which is the new consensus model for Dutch water management. Because this model operates at a scale of 250 by 250 m, dedicated unique combinations can be derived for any given target area. An additional advantage of using this new model would be that all agricultural management practices (land-use, irrigation practices and areas with artificial drainage systems) would be upgraded to the newest available datasets (the current dataset originates from the late 1990s).

Even with the new schematisation, organic matter content will remain uncertain for smaller areas. Furthermore, differences in organic matter content between crops were considerably smaller than in the GeoPEARL version used so far. Given these small differences and the uncertainty in the organic matter content of the soil a specific site, it may be questioned whether assessments for different crops as done in the second tier of the current Decision Tree will give leaching concentrations that are significantly different from each other. We therefore recommend quantifying the uncertainty of model predictions for these smaller crops with the aim to investigate if it is possible to simplify the second tier of the Decision Tree. In addition, the possibility of zooming in on specific areas could be investigated by generating schematisations using different gridcell sizes.

### 7.2.2 Consistency of the tiered approach

The higher leaching concentrations predicted by the GeoPEARL version based on the 2017 soil organic matter map has led to an inconsistency in the tiered approach of the Dutch Decision Tree for leaching to groundwater. This can be corrected by introducing a calibration factor with which the outcome of the first-tier calculations using FOCUS PEARL has to be multiplied. As the leaching for autumn/winter applications is relatively higher than for spring/summer applications, two periods with different calibration factors are recommended, i.e. a factor of 5 for spring/summer applications and a factor of 10 for autumn/winter applications. For a small number of cases (i.e. compounds with a ratio of  $K_{om}/DegT50$  between 3.5 and 4.5), these assessment factors are not high enough. For these cases, it is recommended to skip tier 1 and move directly to tier 2.

The proposed calibration factors are based on calculations for a Freundlich exponent of 0.9. Checks for two substances showed that these calibration factors may not be conservative enough for a Freundlich exponent of 0.8, which is usually the lowest value found in dossiers. To make the tiered approach consistent for all possible substances, we recommend to also estimate the calibration factors for compounds with a Freundlich exponent of 0.8. Consistency of the tiered approach has further not been checked for relevant soil metabolites. It is therefore recommended to also check this.

Depending on the crop, the organic matter content in groundwater abstraction areas can be either lower or higher than in the Dutch agricultural area as a whole. This implies that the 90<sup>th</sup>-percentile of the leaching concentration in groundwater abstraction areas can be either higher or lower than the concentration in the Dutch agricultural area as a whole. This makes it questionable whether the factor of 10 that is currently used to protect groundwater abstraction areas is always necessary. We therefore recommend to systematically compare the predicted leaching concentration in groundwater abstraction areas with that in the Dutch agricultural area as a whole.

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# References

- Adriaanse, P.I., Linders, J.B.H.J., van den Berg, G.A., Boesten, J.J.T.I., van der Bruggen, M.W.P., Jilderda, K., Luttkik, R., Merkens, W.A.W., Stienstra, Y.J., and Teunissen, R.J.M., 2008. Development of an assessment methodology to evaluate the use of plant protection products for drinking water production from surface water. A proposal for the registration procedure in the Netherlands. Alterra Report 165, 246 pp.
- Anonymous, 2015. Proposal for options for specifying the groundwater protection goal at national level within the EU. Available at <http://www.pfmodels.org/emw7.html>, 9 pp.
- Ardia, D., Mullen, K.M., Peterson, B.G. and Ulrich, J., 2015. 'DEoptim': Differential Evolution in 'R'. version 2.2-3.
- Beulke, S. De Wilde, T., Balderacchi, M., Garreyn, F., van Beinum, W., Trevisan, M., 2015. Scenario selection and scenario parameterisation for permanent crops and row crops on ridges in support of predicting environmental concentrations of plant protection products and their transformation products in soil. EFSA supporting publication 2015: EN-813, 170 pp.
- Bilonick, R.A., 1988. Monthly hydrogen ion deposition maps for the northeastern U.S. from July 1982 to September 1984. *Atmospheric Environment* 22, 1909–1924.
- Brus, D.J., De Gruijter, J.J., Marsman, B.A., Visschers, R., Bregt, A.K., and Breeuwsma, A., 1996. The performance of spatial interpolation methods and choropleth maps to estimate properties at points: a soil survey case study. *Environmetrics*, 7, 1-16.
- Cornelese, A.A., Boesten, J.J.T.I., Leistra, M., van der Linden, A.M.A., Linders, J.B.H.J., Pol, J.W.W., and Verschoor, A.J., 2003. Monitoring data in pesticide registration. RIVM report 601450015/2003, RIVM, Bilthoven, 30 pp.
- Cornelese, A.A. and J.W. Pol, Manual for the Authorisation of Pesticides - Plant protection products; Chapter 6 Fate and behaviour in the environment: behaviour in soil; leaching. Version 1.0, 2006.
- De Gruijter, J.J., Brus, D.J., Bierkens, M.F.P. and Knotters, M. 2006. Sampling for Natural Resource Monitoring. Springer, Berlin, Germany.
- De Lange, W.J., G.F. Prinsen, J.C. Hoogewoud, A.A. Veldhuizen, J. Verkaik, G.H.P. Oude Essink, P.E.V. van Walsum, J.R. Delsman, J.C. Hunink, H.Th.L. Massop and T. Kroon, 2013. An operational, multi-scale, multi-model system for consensus-based, integrated water management and policy analysis: The Netherlands Hydrological Instrument. *Environmental Modelling & Software*, 59, 98-108.
- De Vries, F., 1994. A physical-chemical characterisation of the soil-map of the Netherlands, scale 1:50,000. SC-DLO Rep. 256. Alterra, Wageningen, the Netherlands.
- De Vries, F., 1999. Characterizing the soils of the Netherlands according to physical and chemical properties. Report 125, DLO-Staring Centre, Wageningen.
- Dorgelo, F.O. (ed.), 2006. Eindrapportage CTBase. College voor de toelating van bestrijdingsmiddelen, Wageningen.

- 
- EFSA, 2012. Scientific opinion on the science behind the guidance for scenario selection and scenario parameterisation for predicting environmental concentrations in soil. *EFSA Journal* 2012; 10(2):2562. [77 pp.] doi:10.2903/j.efsa.2012.2562.
- EFSA, 2017. EFSA Guidance Document for predicting environmental concentrations of active substances of plant protection products and transformation products of these active substances in soil. *EFSA Journal* 2017, 15(10), 4982.[115 pp.] doi: <https://doi.org/10.2903/j.efsa.2017.4982>
- Finke, P.A., J.J. de Gruijter and R. Visschers, 2001. Status 2001 Landelijke Steekproef Kaarteenheden en toepassingen. Rapport 389, Alterra Wageningen UR.
- FOCUS, 2014. Generic Guidance for Tier 1 FOCUS Ground Water Assessments. Guidance document version 2.2. Available online: <http://esdac.jrc.ec.europa.eu/projects/focus-dg-sante>
- Goovaerts, P., 1997. *Geostatistics for Natural Resources Evaluation*. Oxford University Press, New York.
- Hengl, T., Heuvelink, G.B.M. and Stein, A., 2004. A generic framework for spatial prediction of soil variables based on regression-kriging. *Geoderma*, 120, 75-93.
- Heuvelink, G.B.M. and Bierkens, M.F.P., 1992. Combining soil maps with interpolations from point observations to predict quantitative soil properties. *Geoderma*, 55, 1-15.
- Heuvelink, G.B.M. and Griffith, Daniel A., 2010. Space-Time Geostatistics for Geography: A Case Study of Radiation Monitoring Across Parts of Germany. *Geographical Analysis*, 42, 161-179.
- Hoogland, T., Heuvelink, G.B.M. and Knotters, M., 2010. Mapping Water-Table Depths Over Time to Assess Desiccation of Groundwater-Dependent Ecosystems in the Netherlands. *Wetlands*, 30, 137-147.
- Kempen, B., Brus, D.J., Heuvelink, G.B.M. and Stoorvogel, J.J., 2009. Updating the 1:50,000 Dutch soil map using legacy soil data: A multinomial logistic regression approach. *Geoderma*, 151, 311-316.
- Kempen, B., D.J. Brus and F. de Vries, 2015. Operationalizing digital soil mapping for nationwide updating of the 1:50,000 soil map of the Netherlands. *Geoderma*, 241-242, 313-329.
- Knotters, M., Brus, D.J. and Oude Voshaar, J.H., 1995. A comparison of kriging, co-kriging and kriging combined with regression for spatial interpolation of horizon depth with censored observations. *Geoderma*, 67, 227-246.
- Kovar, K., A. Leijnse, and J.B.S. Gan, 1992. Groundwater model for the Netherlands. *Mathematical Model Development and User's Guide*. RIVM Report 714305002, Bilthoven, the Netherlands.
- Kovar, K., M.J.H. Pastoors, A. Tiktak and F.W. van Gaalen, 1998. Application of the Netherlands Groundwater Model, LGM, for calculating concentration of nitrate and pesticides at abstraction wells in sandy soil areas of the Netherlands. RIVM Report 703717002, Bilthoven, the Netherlands.
- Kruijne, R., Tiktak, A., Van Kraalingen, D., Boesten, J.J.T.I., and A.M.A van der Linden, Pesticide leaching to the groundwater in drinking water abstraction areas, Analysis with the GeoPEARL, Alterra-report 1041.doc, Alterra, Wageningen, 2004  
<https://www.wageningenur.nl/nl/Publicatie-details.htm?publicationId=publication-way-333334373735>
- KWR, 2012. Verzamelen gegevens grondwateronttrekkingen Nederland. Rapport KWR 2012.050 Watercycle Research Institute, Nieuwegein, The Netherlands.

- 
- McBratney, A.B. and Webster, R., 1981. The design of optimal sampling schemes for local estimation and mapping of regionalized variables II. Program and examples. *Computers & Geosciences* 7, 335-365
- Mullen, K., Ardia, D. Gil, D., Windover, D., and Cline, J., 2011. 'DEoptim': An R Package for Global Optimization by Differential Evolution. *Journal of Statistical Software*, 40(6), 1-26. URL <http://www.jstatsoft.org/v40/i06/>.
- NEN, 2014. Soil - Determination of organic matter content on a mass basis in soil and sediment as loss-on-ignition. NEN 5754, NEN, Delft, The Netherlands.
- Reijneveld, A., Wensem, J. van, and Oenema, O., 2009. Soil organic carbon contents of agricultural land in the Netherlands between 1984 and 2004, *Geoderma* 152, 231-238.
- Sleutel, S., De Neve, S., Singier, B. and G. Hofman, 2007. Quantification of Organic Carbon in Soils: A Comparison of Methodologies and Assessment of the Carbon Content of Organic Matter. *Communications in Soil Science and Plant Analysis*, 38, 2647 -2657.
- Storn, R. and Price, K., 1997. *Journal of Global Optimization* 11: 341. doi:10.1023/A:1008202821328
- Tiktak, A., de Nie, D.S., Piñeros Garcet, J.D., Jones, A., Vanclooster, M., 2004. Assessment of the pesticide leaching risk at the Pan-European level. The EuroPEARL approach. *Journal of Hydrology*, 289, 222-238.
- Tóth, G., Jones, R.J.A. and Montanarella, L., 2013. LUCAS Topsoil Survey. Methodology, data and results. Joint Research Centre Technical Reports EUR 26102 EN, Office for Official Publications of the European Communities, Luxembourg.
- Uffink, G.J.M., and van der Linden, A.M.A., 1998. Dilution of pesticides in groundwater during advective dispersive transport. RIVM report 716601002.
- Van den Akker, J.J.H., T. Hoogland, A.H. Heidema, 2008. Maaiveld daling en drooglegging in Groot Mijdrecht nu en in de toekomst, *Alterra-Rapport 1734*, Wageningen
- Van den Berg, F., Tiktak, A., Heuvelink, G.B.M., Burgers, S.L.G.E., Brus, D., De Vries, F., Stolte, J. and J.G. Kroes, 2012. Propagation of uncertainties in soil and pesticide properties to pesticide leaching, *Journal of Environmental Quality*, 41, 253-261.
- VanderBorgh, J., A. Tiktak, J.J.T.I. Boesten and H. Vereecken, 2011. Effect of pesticide fate parameters and their uncertainty on the selection of 'worst-case' scenarios of pesticide leaching to groundwater. *Pest Management Science* 67, 294-306.
- Van der Linden, A.M.A., Boesten, J.J.T.I., Cornelese, A.A., Kruijne, R., Leistra, M., Linders, J.B.H.J, Pol, J.W., Tiktak, A. and A.J. Verschoor, The new decision tree for the evaluation of pesticide leaching from soils., RIVM report 601450019/2004, RIVM, 2004 <http://www.rivm.nl/bibliotheek/rapporten/601450019.pdf>
- Visschers, R., P.A. Finke and J.J. de Gruijter, 2007. A soil sampling program for the Netherlands. *Geoderma*, 139, 60-72.
- Walkey, A. and Black, I.A., 1934. An examination of the Degtjareff method for determining soil organic matter, and a proposed modification of the chromic acid titration method. *Soil Science*, 34, 29-38.

# Annex 1 DegT50 and K<sub>om</sub> values of test substances

Substance	DegT50	K <sub>om</sub>	Substance	DegT50	K <sub>om</sub>	Substance	DegT50	K <sub>om</sub>
1	20	0	41	20	80	81	20	160
2	40	0	42	40	80	82	40	160
3	60	0	43	60	80	83	60	160
4	80	0	44	80	80	84	80	160
5	100	0	45	100	80	85	100	160
6	120	0	46	120	80	86	120	160
7	140	0	47	140	80	87	140	160
8	160	0	48	160	80	88	160	160
9	180	0	49	180	80	89	180	160
10	200	0	50	200	80	90	200	160
11	20	20	51	20	100	91	20	180
12	40	20	52	40	100	92	40	180
13	60	20	53	60	100	93	60	180
14	80	20	54	80	100	94	80	180
15	100	20	55	100	100	95	100	180
16	120	20	56	120	100	96	120	180
17	140	20	57	140	100	97	140	180
18	160	20	58	160	100	98	160	180
19	180	20	59	180	100	99	180	180
20	200	20	60	200	100	100	200	180
21	20	40	61	20	120	101	20	200
22	40	40	62	40	120	102	40	200
23	60	40	63	60	120	103	60	200
24	80	40	64	80	120	104	80	200
25	100	40	65	100	120	105	100	200
26	120	40	66	120	120	106	120	200
27	140	40	67	140	120	107	140	200
28	160	40	68	160	120	108	160	200
29	180	40	69	180	120	109	180	200
30	200	40	70	200	120	110	200	200
31	20	60	71	20	140	111	20	250
32	40	60	72	40	140	112	40	250
33	60	60	73	60	140	113	60	250
34	80	60	74	80	140	114	80	250
35	100	60	75	100	140	115	100	250
36	120	60	76	120	140	116	120	250
37	140	60	77	140	140	117	140	250
38	160	60	78	160	140	118	160	250
39	180	60	79	180	140	119	180	250
40	200	60	80	200	140	120	200	250





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