CCAT

Cross Compliance Assessment Tool

CROSS-COMPLIANCE ASSESSMENT TOOL

Policy-oriented research:
Scientific support to policies SSP

Specific Targeted Research Project (STREP)

Deliverable(s): 4.2.3.2

Derivation of DNDC meta-models to evaluate the impact of cross compliance measures on nitrogen N surplus, N leaching, N2O emissions at EU25 scale

Due date of deliverable: [01-01-2009]

Actual submission date: [25-09-2009]

CROSS-COMPLIANCE ASSESSMENT TOOL
EC contract number 44423-CCAT
Project duration: January 2007-December 2009

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Disclaimer:

“This publication has been funded under the CCAT project, EU 6th Framework Programme, Priority 8.1 (European Commission, DG RTD, contract no. 44423-CCAT). Its content does not represent the official position of the European Commission and is entirely under the responsibility of the authors.”

Project co-funded by the European Commission within the Sixth Framework Programme (2002-2006)		
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Contents

Executive summary

Agriculture is a multi-goal system since it has to meet the increasing demands in food and fibers, while continuing to preserve the surrounding environment. The Cross-Compliance (CC), introduced into the last 2003 CAP revision, aims to push the farmers into adopting more sustainable agricultural practices as prerequisite to receive direct payments.

The Cross-Compliance Assessment Tool (CCAT) develops an integrated simulation platform to quantify the effects of CC measures by means of environmental indicators.

Our CAPRI/Europe-DNDC metamodeling approach reduces the running time and memory consumption of the original DNDC code; it has been integrated into CCAT to estimate the N2O emission, N leaching and N surplus, according to few pre-selected CC scenarios. The metamodels are implemented in R computing environment by using the Random Forest package.

1 Introduction

The Common Agricultural Policy (CAP) introduced a compulsory Cross-Compliance (CC) tool to check up the respect of several environmental, food safety, animal welfare, and animal and plant health standards (SMRs) as well as the maintenance of farmlands in good agricultural and environmental condition (GAECs), as prerequisite for receiving direct payments. However nowadays it still remains quite difficult to quantify the effect of this compulsory cross-compliance by means of indicators. To address this topic the CCAT project aims to develop a simulation platform integrating different models to provide an exhaustive cost and benefits analysis of CC at the European scale, helping the environmental policy makers to better understand complex and dynamic systems and to face future issues.

Our CAPRI/Europe-DNDC modeling approach have been included into the CCAT to estimate several environmental indicators, such as N2O emissions, N leached and N surplus, according to selected agro-environmental measures and different agricultural land uses.

2 Materials and Methods

2.1 Introduction

The frequent use of simulation based models for analyzing of complex phenomena is changing the traditional approaches to environmental and hazard problems. The continuous improvement of computer performance allows for more detailed mathematical representations, based on space-time discretisation, to be developed and run to describe, in quantitative manner, complex real systems, reproducing the way their spatial patterns evolve and the relationships of physical processes and socio-economic developments [Follador et al., 2008].

To assess the CC effects on the European environment a modeling framework that integrates the agro-economical CAPRI model with the biogeochemical model Europe-DNDC, have been developed. While CAPRI simulates how the socio-economical aspects impact on land use and farm management, DNDC uses these information and other physical parameters to estimate the selected environmental indicators such as N2O emission, N leached, N surplus from agricultural soils (Fig 1).

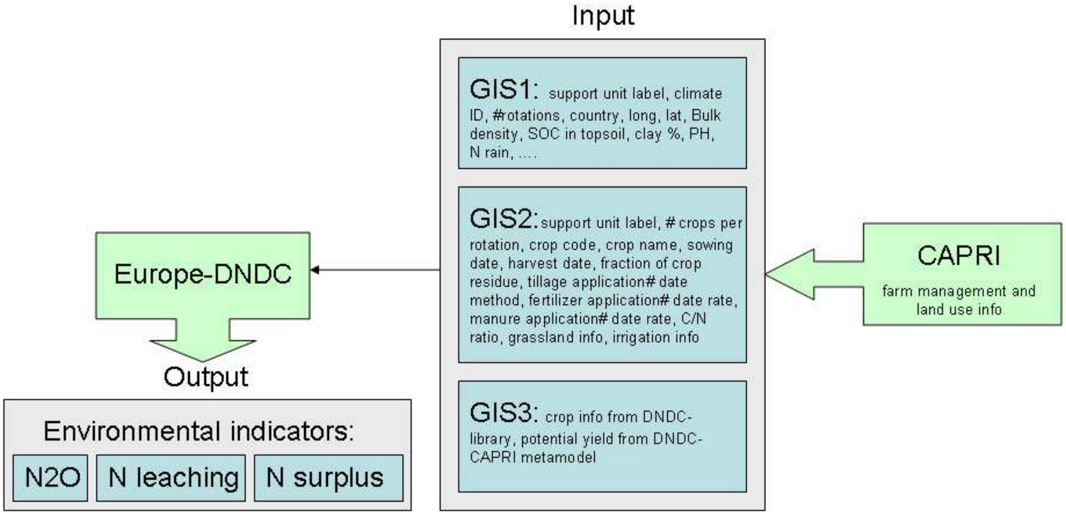

Figure 1: simplified framework of CAPRI/Europe-DNDC modeling approach

2.2 Europe-DNDC description

The original Denitrification-Decomposition model (DNDC) [Li et al., 2000], a process-oriented biogeochemistry model for agro-ecosystems, is a mechanistic detailed model specifically created for using at field level, but subsequently developed to be applied at regional scale. DNDC simulates the carbon trend, the nitrogen balance and trace gas emissions from agricultural soils. It is comprised of two components which integrate ecological drivers (e.g., climate, soil, vegetation, etc.) and soil environmental factors (e.g., temperature, PH, etc.) on one hand, and soil environmental factors and soil biogeochemical reactions on the other hand [Li et al., 2006]. The first component consists of 3 submodels (soil climate, crop growth and decomposition); it calculates the state of soil-plant system such as soil physical and chemical status, vegetation growth and organic carbon mineralization. The second component is comprised of nitrification, denitrification and fermentation submodels; it predicts the main processes involved in the GHGs production, by using the soil environmental data.

Europe-DNDC partially modifies/integrates the original DNDC code to adapt it to our applications, allowing a more flexible simulation of a large number of spatial-agricultural units and including the possibility to select up to ten different crops to be simulated into a specific simulation unit [Leip et al., 2008].

2.3 HSMU support

The HSMU (Homogeneous Spatial Mapping Unit) is the minimal geographical unit used for the spatial simulation. The Europe of 25 Member States is composed by 207439 HSMUs which are multipart polygons derived from the overlay of four different datasets: administrative boundaries (Gisco NUTS2 e NUTS3), land cover

(CORINE level 3), soil (SGDB classification) and slope data (CCM DEM 250 divided in five classes).

The main environmental (meteorological and soil datasets) and social-economic (farm management) parameters are extracted at HSMU level performing zonal statistic or crosstab analysis. The meteorological data (temperature, precipitation, relative humidity, evaporation, global radiation) at 1x1 km spatial resolution and daily temporal resolution from 1901-2000 [Orlandini and Leip, 2008] has been obtained combining MARS grid weather data (interpolated daily weather data at 50x50 km spatial resolution) with the ATEAM/CRU data (interpolated monthly climate data at 10'x10' spatial resolution). The soil information such as initial SOC, clay content, etc. were obtained from the 1x1 km^2 soil raster datasets, processed on the basis of the European Soil Database [Jones et al., 2005]. The soil database was re-sampled using a mask for annual crops and gap-filled to eliminate bias in the parameters due to inconsistent land-use information. Some important farm management parameters at HSMU level, such as organic and mineral N application rates, and crop yield, derive from the spatial disaggregation of the information estimated by CAPRI at NUTS 2 level (regional database) [Leip et al., 08].

2.4 Farming management scenario conceptualization

Even though the SMRs and GAECs are country or even region specific, we generalized some of these measures across the EU25 Member States, according to the practical feasibility and implementation into our modeling approach. In this contribution we only present the results for corn crops. To reduce the time and memory consumption, also considering the number of scenarios (7) and the length of the period (1990-99) to simulate, we decided to select a representative sample subset among the entire EU25 agricultural lands. The final HSMU set (about 20000) has been chosen by applying a minimum threshold in land use (percentage of corn crops on HSMU agricultural land > 10%).

The definition of scenarios is necessary whenever we want to compare the estimated agricultural activities' effects under CC vs. the conventional practices, to carry out a cost-benefit analysis in terms of ecosystem preservation, yield, market competitiveness, soil fertility, GHG emission, etc. This first assessment should provide a deeper knowledge of European agro-environmental policy impact, offering a more exhaustive overview for future plans.

2.4.1 Corn-Reference scenario (S1)

The baseline scenario includes only a corn monoculture, with one tillage application and a tillage depth of 20cm. The simulated period is 10 years of no irrigated corn, without rotations or fallow, within the previously selected HSMUs. We apply both fertilizer (1) and manure (2) N inputs, per year. The second manure spreading includes the green manure (residue). The fertilizer N input is set to 0 during the winter. Other N inputs are atmospheric deposition, biological fixation and root residue.

2.4.2 Corn-No till scenario (S2)

The no tillage scenario differs from the reference scenario in the absence of tillage application. This practice of turning the soil before planting buries crop residues, animal manure and troublesome weeds and also aerates and warms the soil. But it can also increase the soil vulnerability to erosion by wind and water [Huggins et al., 2008]. No till farming in contrast try to minimize soil disruption and have been suggested to increase carbon storage in soils (GAEC02: surface protection).

2.4.3 Corn-Max Manure scenario (S3)

This scenario limits the N in manure spreading to 170 kg N/ha y^{-1} (with few exceptions), compared to the reference scenario. (SMR04: restriction of organic manure application).

2.4.4 Corn-Catch crop scenario (S4)

In this scenario we simulate two cycles of corn-alfalfa cropping system. One cycle is comprised of a rotation between a yielding crop (corn) for 2 years, and a catch crop (alfalfa) which lasts 3 years. We selected alfalfa because of its well known ability to fix N in the soil. The corn crop receives both fertilizer (1) and manure (2) applications, and it is tilled at 20 cm depth. We apply one manure spreading without tillage on the catch crop. (GAEC01, GAEC02: surface protection; maintenance of Soil Organic Matter-standard for crop rotation).

2.4.5 Barley -Reference scenario (S5)

The baseline scenario is the same as S1 with Barley instead of corn, i.e. a barley monoculture, with one tillage application and a tillage depth of 20cm. The simulated period is 10 years of no irrigated barley, without rotations or fallow, within the previously selected HSMUs (see further S1). We apply both fertilizer (1) and manure (1) N input. Other N inputs are atmospheric deposition, biological fixation and root residue.

2.4.6 Barley --No till scenario (S6)

The no tillage scenario differs from the reference scenario in the absence of tillage application. This practice of turning the soil before planting buries crop residues, animal manure and troublesome weeds and also aerates and warms the soil. But it can also increase the soil vulnerability to erosion by wind and water [Huggins et al., 2008]. No till farming in contrast try to minimize soil disruption and have been suggested to increase carbon storage in soils (GAEC02: surface protection). This scenario is the same as S2 with Barley instead of corn.

2.4.7 Barley --Max Manure scenario (S7)

This scenario limits the N in manure spreading to 170 kg N/ha y^{-1} (with few exceptions), compared to the reference scenario. (SMR04: restriction of organic manure application). This scenario is the same as S3 with Barley instead of corn

Table 1: Description of scenarios and measures related to SMRs and GAECs in Europe-DNDC approach

SMR	Name	Description	DNDC scenario and parameterisation
SMR2	Maximum manure N application standard	The amount of applied N in manure and excreted during grazing may not exceed 170 kg N per ha in a region. Excess manure is transported or processed.	Comparison of S1: Corn Reference Scenario1 with S3: Corn Max Manure scenario[2] Comparison of S5: Barley reference scenario[1] with S7: Barley max manure scenario[2]
SMR8	Growing winter crops	Growing catch crops will result in i) less N leaching below rooting zone, ii) less surface runoff, and iii) less requirement of fertilizer N in the following year.	Comparison of S1: Corn Reference Scenario with S4: Corn Catch crop scenario[3]
GAEC	**Name**	**Standards**	**DNDCD scenario and parameterisation**
GM3	Minimum coverage-arable land	Vegetative cover between agricultural crops, which is then ploughed into the soil, also termed as catch crops, green manure and winter crops.	Comparison of S1: Corn Reference Scenario with S4: Corn Catch crop scenario[3] Actually equal to SMR8
GM4	Tillage method	Zero tillage	Comparison of S1: Corn Reference Scenario with S2: Corn No tillage Scenario[4] Comparison of S5: Barley reference scenario with S6: Barley No tillage scenario[4].

[1] The baseline scenario includes only a corn or barley monoculture, with one tillage application and a tillage depth of 20cm

[2] This scenario limits the N in manure spreading to 170 kg N/ha y^{-1} (with few exceptions), compared to the reference scenario.

[3] Catch crops scenario includes two cycles of corn-catch crop system which lasts 5years (2 years of corn + 3 years of alfalfa). Corn like baseline, alfalfa without tillage and fertilizer application

4 The no tillage scenario differs from the reference scenario because of the absence of tillage

3 CAPRI/Europe-DNDC output

3.1 S2 vs. S1

The prediction by Europe-DNDC models (Fig 2) indicates that conversion from conventional tillage to no tillage results in a general reduction of N2O emission, even though an increase is pointed out for a group of HSMU. This different behavior can be explained by considering the different water soil contents and texture across EU. [Grant et al., 2004] show how tillage may lead to more nitrification (and thus more N2O) in drier soil, by increasing decomposition of organic matter. In the soil with higher soil water, and thus a reduced air-filled porosity, the no-till results in high N2O flux due to the enhancement of denitrification [Ball et al., 1999]. [Rochette, 2008] try to generalized these conclusions; he shows as no-till generally increase N2O emissions in poorly aerated soil, while its impact in soil with good and medium aeration is neutral or positive. Our results covering the whole EU25 territory showed that a conversion to no-till leads to a reduction of N2O of 20% on the entire subset, compared to the baseline scenario.

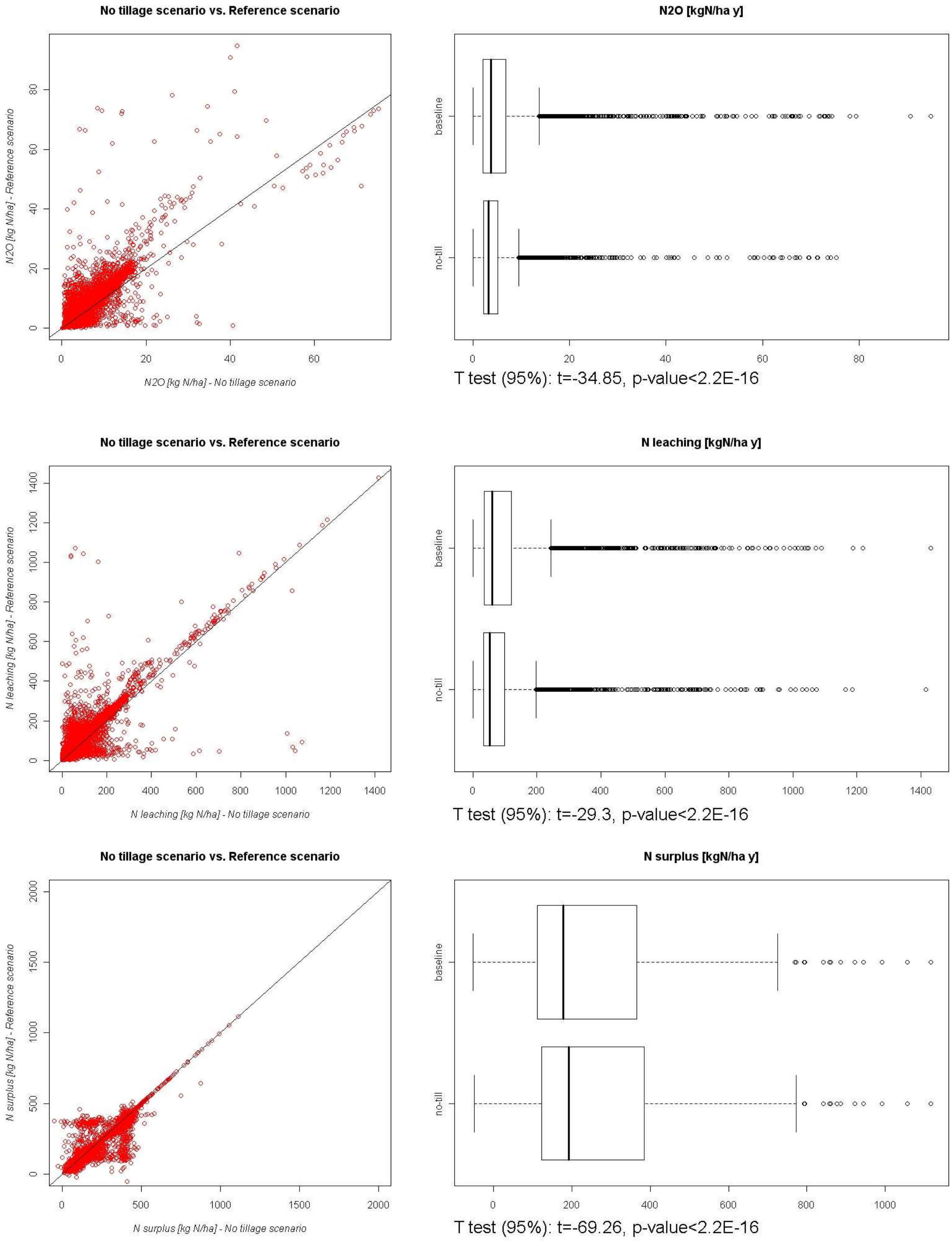

Figure 2: Corn - No-till scenario vs. Baseline scenario: N2O, N leaching and N surplus. In the left panels: scattergrams of environmental indicators, no-till vs. baseline scenario. In the right panels: boxplot of environmental indicators, no-till vs. baseline scenario. The t value (paired-T test) points out the big difference between the no-till scenario output and the baseline scenario output; the very little p-value confirms the significativity of this difference.

The N ($NO3^-$) leaching from fields is directly controlled by hydrogeological and plant-soil processes, both influenced by numerous factors such as climate conditions, soil properties and farming management (tillage method, fertilization, crop rotations, etc.). The simulated output indicates that the conversion of conventional tillage to no-till decreases the N leaching loss (-13%). This result can be explained by means of N mineralization reduction, resulting in increased SOC and less inorganic N available for leaching [Farahbakhshazad et al., 2008].

The N surplus slightly increases in the no-tillage scenario (+6%); as the manure and fertilizer N input are the same of the baseline scenario, this difference has to be explained by means of the other N sources considered for the N surplus calculation. The conversion from tillage to no till caused a diminution of plant uptake and N input from root residue, and a slightly increase in N fixation. The reduction in plant uptake can require the use of extra nitrogen fertilizer to meet the nutritional needs of some crops, because increasing organic matter at the surface immobilizes nutrients, including nitrogen [Huggins et al, 2008].

3.2 S3 vs. S1

We split the manure amendment to 2 applications; the second one includes the green manure (residue). The tillage turns the soil before planting and buries the manure, limiting the losses occurring after application, such as NH3 volatilisation, $NO3^-$ leaching and denitrification [Salazar et al., 2004].

By applying a maximum threshold of 170 kgN/ha y^{-1} in the first organic N input[1], we reduced the environmental impact of corn cropping systems. The estimated indicators (Fig 3) show a decrease of N2O (-24%), N leaching (-14%) and N surplus (-15%). This scenario could introduce new additional costs for enlarging the place to store the manure, for those farmers used to spread it as litter [Follador et al, 2009].

[1] This threshold is not applied to green manure – our second amendment.

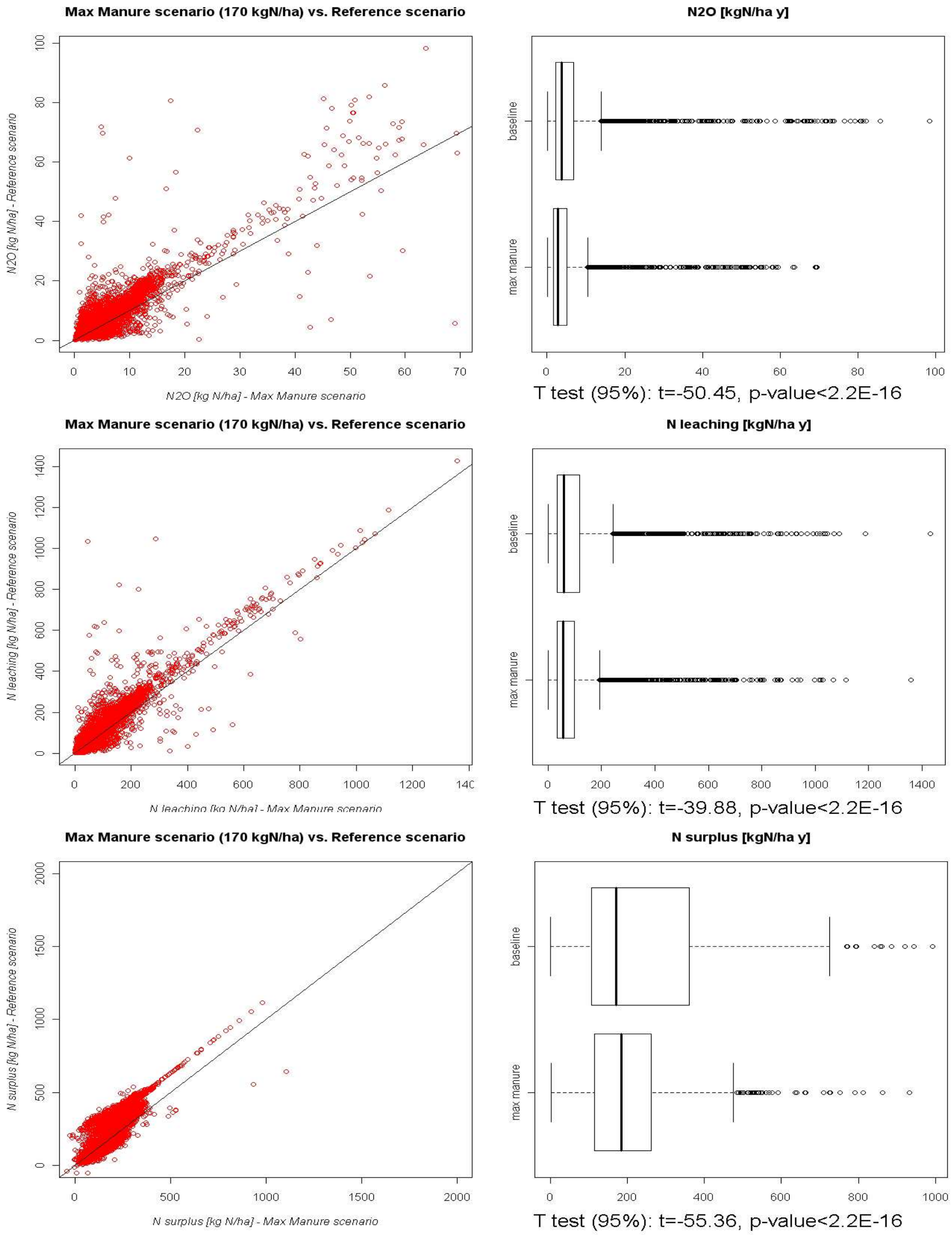

Figure 3: Corn - Max manure scenario vs. Baseline scenario: N2O, N leaching and N surplus. In the left panels: scattergrams of environmental indicators, Max manure vs. baseline scenario. In the right panels: boxplot of environmental indicators, max manure vs. baseline scenario. The t value (paired-T test) points out the big difference between the max manure scenario output and the baseline scenario output; the very little p-value confirms the significativity of this difference.

3.3 S4 vs. S1

Growing catch/break crops, under no-till, is one of the best practices of conservative agriculture [FAO, 2005] and it completely replaces the set-aside from 2008. Its well known benefits include: (a) prevention of erosion by anchoring soil and lessening the impact of raindrops; (b) reduced risk of deep drainage; (c) more efficient use of water; (d) add plant material to the soil for organic matter recovery; (e) some plants, especially leguminous species, increase the N fixation.

Moreover, in comparison with the reference scenario, the catch crop scenario (Fig. 4) reduced the N2O emission (-27%), the N leaching (-20%) and the N surplus (-34%). These results are the obvious consequence of reduced N input from fertilization and manure amendment on the no-tilled alfalfa and of the increased N fixation capacity of this crop.

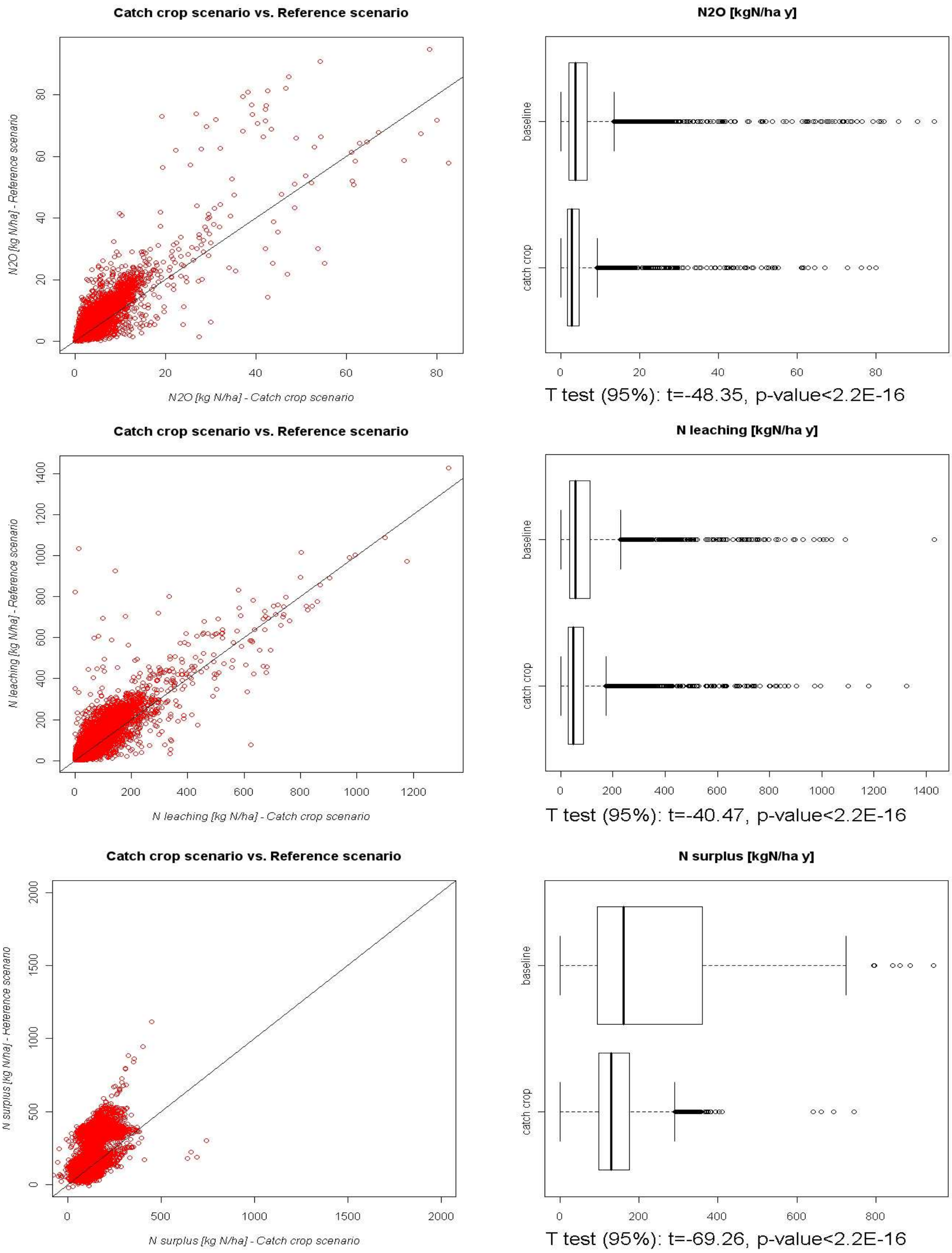

Figure 4: Corn - Catch crop scenario vs. Baseline scenario: N2O, N leaching and N surplus. In the left panels: scattergrams of environmental indicators catch crop vs. baseline scenario. In the right panels: boxplot of environmental indicators, catch crop vs. baseline scenario. The t value (paired-T test) points out the big difference between the catch crop scenario output and the baseline scenario output; the very little p-value confirms the significativity of this difference.

3.4 S6 vs. S5

Compared with the previous Corn-scenarios, the differences between reference and alternative managements are less evident, pointing out how these conservative measures did not considerably affect the environmental indicators' estimation on the barley HSMU subset.

Once more, the conversion from conventional tillage to no tillage (Fig.5) results in a general slight reduction of N2O emission (-4%). As formerly remarked, the N2O emission across the European farmlands strictly depends on the soil texture and water contents; [Rochette, 2008] he showed as no-till generally increase N2O emissions in poorly aerated soil, while its impact in soil with good and medium aeration is neutral or positive.

The N ($NO3^-$) leaching from fields is directly controlled by hydrogeological and plant-soil processes, both influenced by numerous factors such as climate conditions, soil properties and farming management (tillage method, fertilization, crop rotations, etc.). The simulated output indicates that the conversion of conventional tillage to no-till slightly reduced N leaching loss (-2.45%) on the barley subset.

The N surplus didn't change in the no-tillage scenario (-0.006%). We observed a diminution of plant uptake and N input from root residue, and an increase in the N fixation.

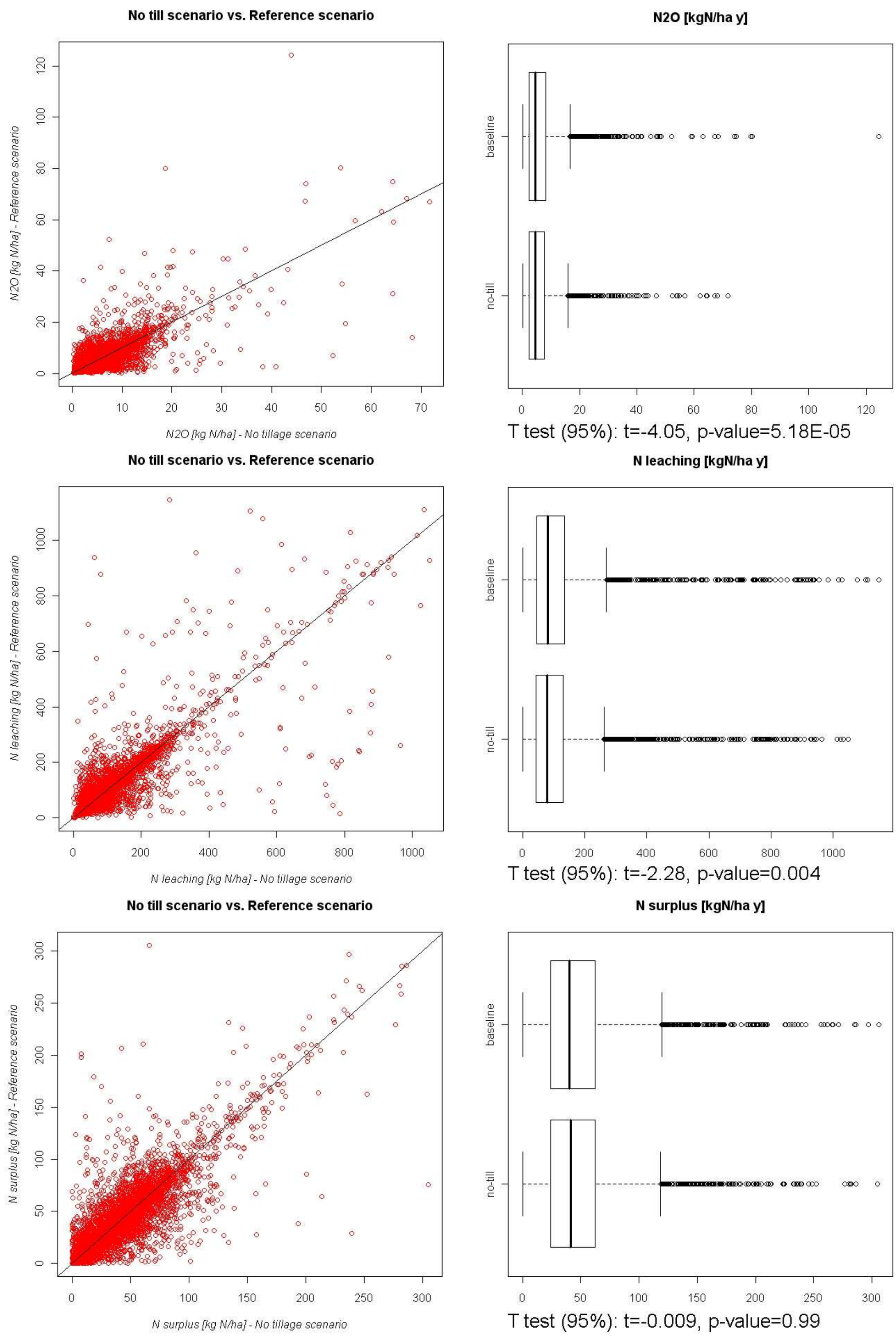

Figure 5: Barley - No till scenario vs. Baseline scenario: N2O, N leaching and N surplus. In the left panels: scattergrams of environmental indicators no till vs. baseline scenario. In the right panels: boxplot of environmental indicators, no till vs. baseline scenario. The t value (paired-T test) points out the difference between the N2O e N leaching in no till scenario output and the baseline scenario output; the little p-value confirms the significativity of this difference. The N surplus outputs don't show significant differences.

3.5 S7 vs. S5

The number of HSMUs with a manure amendment > 170 kg/ha y^{-1} is quite small. Consequently the impact of this measure is not as evident as in the previous corn cropping systems. The tillage turns the soil before planting and buries the manure, limiting the losses occurring after application, such as NH3 volatilisation, $NO3^-$ leaching and denitrification [Salazar et al., 2004].

By applying a maximum threshold at the organic N input, we have observed a slight decrease in all environmental indicators (Fig.6): N2O (-1.7%), N leaching (-0.07%) and N surplus (-3%). This scenario could introduce new additional costs for enlarging the place to store the manure, for those farmers used to spread it as litter [Follador et al, 2009].

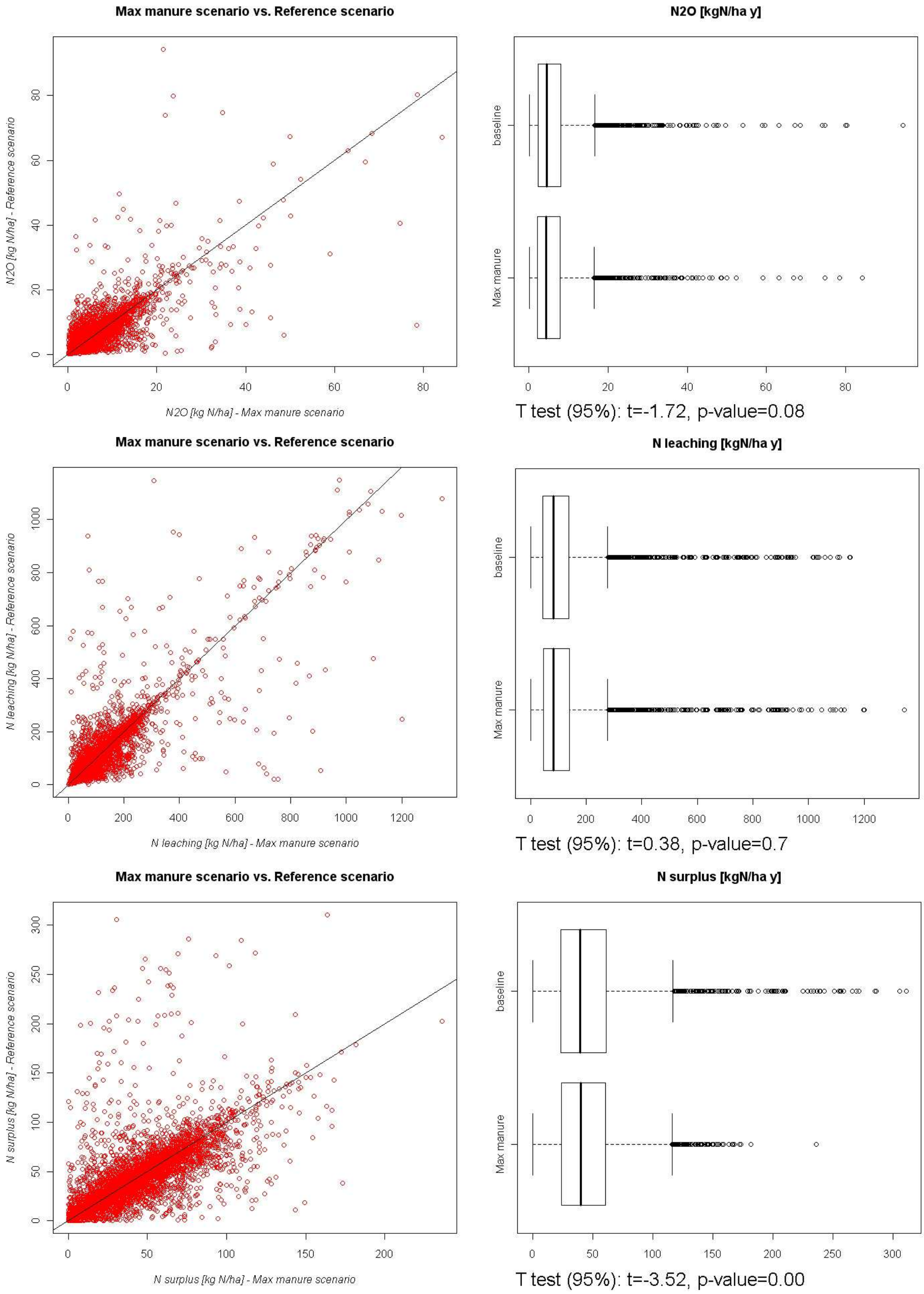

Figure 6: Barley - Max manure scenario vs. Baseline scenario: N2O, N leaching and N surplus. In the left panels: scattergrams of environmental indicators, Max manure vs. baseline scenario. In the right panels: boxplot of environmental indicators, max manure vs. baseline scenario. The T test analysis point out the very little differences between the max manure and reference outputs.

4 Metamodeling

4.1 Introduction

The using of metamodel to approximate expensive computer analysis codes knows today an increasing application in many disciplines. A metamodel can be considered as a model of a model, i.e., a statistical approximation or a simplified description of a complex system by means of computer codes [Simpson et al., 2001].

Despite the great powers of modern calculators, many models require a long running time and a large memory space to compute the responses vector. The use of deterministic modeling at macro-scale applications is often prohibited, because of computational needs and parameterization constraints [Pineros et al., 2005].

At the same time the functional relationship between input and output could be not clear and hidden behind a complex, long and sometime confused computer code.

Statistical techniques are widely used to simplify this analysis by reducing time and memory consumption and underlining the cause-effect connection between predictors (x) and responses (y).

If we represent the original model (e.g., DNDC) through the functional relationship:

$$y=f(x) \qquad [1]$$

its approximation will be

$$y^{*}=f_{m}(x), \text{ so that } y=y^{*}+E \qquad [2]$$

where E is an error term including both the random and metamodel fitting errors.

Typically the construction of a metamodel "f_m" involves the following steps: (1) choose a subset of input variables to feed the metamodel and generate data. (2) Choose the mathematical form of "f_m". (3) Design the calibration and validation sets from the previously selected subset. (4) Fitting the metamodel to the observed data by means of training and test.

The metamodelling process in general decreases the dimensionality of the problem by reducing the number of factors (design variables) used by the original model. This screening out step considers only the most important predictors for a specific application among all the x elements.

4.2 Metamodels development

Among the numerous statistical methods existing in the engineering design literature, we decided to focus on 3 models to represent our data: (a) Neural Network, (b) Support Vector Machine and (c) Random Forest. All these approaches are well designed for complex and non-linear systems; moreover they are able to process a large volume of information. In order to perform the analysis with the best suited approach, we first performed a model comparison. We first provide a short description of the three models, dedicating slightly more attention to the Random Forests which proved to show the best performance (see section 4.3) and has been selected to be used in our project.

4.2.1 A rapid overview on Neural Networks (NN)

An artificial neuron is the basic unit of Neural Networks (NN) and it is comprised of 3 elements (Fig 5):

- ✓ An input layer with a specific number of input cells "$(x_i)_{i=1\ldots m}$".
- ✓ A net of synapses and connections, characterized by weights "$(w_i)_{i=0\ldots m}$". the inputs will be integrated by means of additive function "Σ".
- ✓ An output node which stores the answer of the neuron to the stimulus. It is the result of the weighted integration of inputs, limited by an activation function "g".

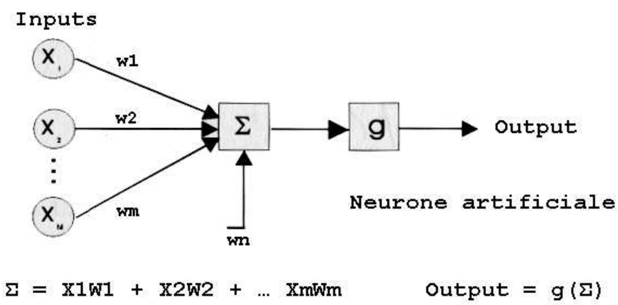

Figure 7: Simplified graphical description of an artificial neuron [Follador, 2008]

A neuron can be described as follows [Follador, 2008]:

$$\begin{cases} v_k = \sum_{j=1}^{m} w_{kj} x_j + w_{0k} \\ y_k = \varphi(v_k) \end{cases} \qquad [3]$$

where "w_{ok}" is called bias and "φ" is the sigmoid (activation function) we used.

The neural networks (NN) are parallel computational models composed of a group of densely interconnected adaptive processing units, called neurons (Fig 6) The disposition and the number of cells, synapses and hidden layers define the topology of the NN.

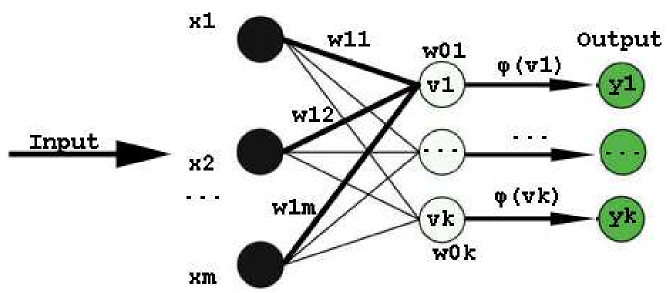

Figure 8: Graphical representation of Neural Networks. It is comprised of one input layer, a series of weighted synapses between cells, hidden layers and one output layer [Follador, 2008].

NN are adaptive models which learn by examples. Here we developed a Multilayer Perceptron (MLP), the most famous class of feedforward NN with supervised training [Follador, 2008; Kanevski et al., 2004]. The MLP is composed by one hidden layer and learns through a backpropagation algorithm. The best net minimizes the MSE between real output (i.e., DNDC-EU output) and the predicted ones [Follador et al., 2008; Villa et al., 2007] The R package *nnet* [Venables et al., 1999] was downloaded and implemented in our metamodel to carry out the training-optimization step.

For further information on neural networks we refer the reader to the suggested references.

4.2.2 A rapid overview on Support Vector Machine (SVM)

The Support Vector Machine has been introduced by [Boser et al., 1992] and was originally designed to address classification problems. Afterwards [Vapnik, 1995] applied the SVM to regression problems; it has proven to be a powerful and robust methodology for learning from empirical data.

We suppose to have a random pair (X,Y), where X is the vector of explanatory variables and Y is the vector of real output value. We are given a learning set of "n" i.i.d.[2] observations of (X,Y): $(x_i,y_i)_{i=1\ldots n}$, to define and train the learning machine. The aim is to predict the target variable from the input set according to a few minimization-optimization steps.

We used a SVM regression with a Gaussian kernel, so that 3 parameters had to be tuned by means of the *tune.svm* function (cross-validation) included into the e1071 R package: 1) "ϵ" of the loss function, 2) the regularization parameter "C", 3) the Gaussian Kernel parameter "γ".

[2] i.i.d. : independent and identically distributed.

Due to the complexity of this approach, we skip the theoretical formulation, and let to the readers the possibility of consulting the recommended references.

4.2.3 A rapid overview on Random Forest (RF)

Random Forest is an aggregation of binary regression trees, a statistical method for regression function estimation, and a learning method, the bagging, based on a random combination of numerous regression functions [Villa, 2009].

In bagging each tree growths independently from the other ones by using a bootstrap sample[3] of the data set [Liaw et al, 2002]. At the end it averages the estimates of regression function out, obtained from the boostrap samples; the general steps could be resumed as follows:

- ✓ Create the bootstrap samples ζ_b , where b=1,…,B replica
- ✓ Calculate the regression tree ψ_b* estimated from ζ_b
- ✓ Estimate ψ(x) for all (x):

$$\psi(x) = \frac{1}{B}\sum_{b=1}^{B}\psi_b *(x) \qquad [4]$$

[Breiman, 2001] add some improvements to this algorithm:

1) An "out of bag" error is calculated at each step (B is growing). It represents the mean of the errors of each estimator on the data not used to build it (not in ζ_b):

$$OOB = \sum_{b=1}^{B} \sum_{i:(x_i,y_i)\notin\zeta_b} (\psi_b *(x_i) - y_i)^2 \qquad [5]$$

   The OOB helps to prevent the overfitting and stops the algorithm once stabilized.

2) A layer of randomness: for each node the best split is carried out by using a subset of randomly selected "q" predictors. An advisable choice is q=√p into the whole set of $(X_i)_{i=1\ldots p}$ predictors. In this way the regression function ψ_b*(x) becomes more robust to outliers and noise, and performs very well compared to many other classifiers.

The random Forest is very user-friendly and easily parallelized. Moreover it provides useful information about the estimate of error and the variable importance. To calculate the last one, the value of the variable is randomly permutated and the loss in MSE compared to the original value, is stored. The bigger this loss, the most important is the predictor for the output estimation (see Annex 1).

[3] The dataset is composed of $(X,Y)_{i=1\ldots p}$ couples of random variables, where X includes both quantitative or qualitative predictors and Y is the quantitative variable to be predicted by using X. The boostrap subsample is a random sample with replacement in "n" observation of (X, Y). In RF we create B boostrap samples to train the model.

As showed in Fig. the forest error converges to a limit as the number of trees into the forest becomes large (e.g., 500).

4.3 Metamodels' performance comparison

From the original predictors vector x we screened out the less important ones for the estimation of the studied environmental indicators; the final set is composed of $(x,y)^s$ selected couples.

The calibration subset include 80% of these input/output data $(x_i, y_i)^s$, randomly selected, while the validation has been based on the remaining 20%.

The first results of the training and testing phases have been used to assess the metamodels behaviors; by comparing their performances we have been able to choose the best statistical method for our application (Fig 7).

The error during the calibration and validation was calculated comparing the true output "y=f(x)" (estimated by DNDC-EU) vs. the values predicted by the metamodel "$y^*=f_m(x^s)$".

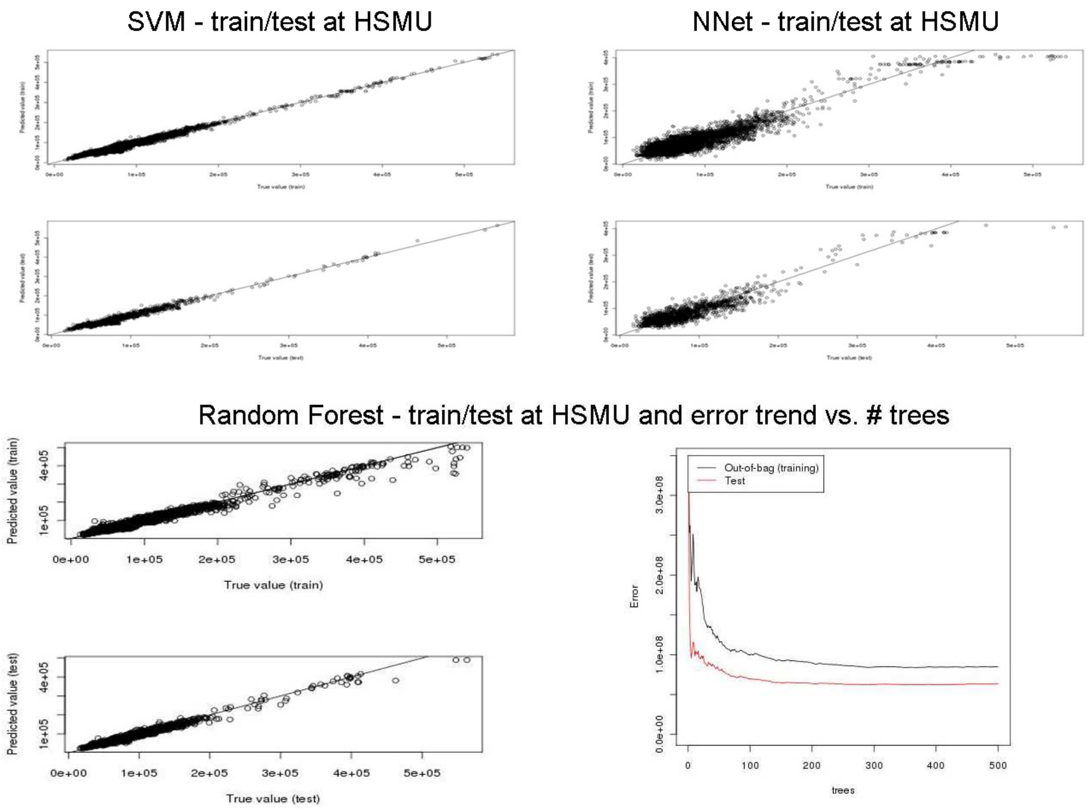

Figure 9: metamodels' performance at HSMU level. Both train and test steps are displayed. We selected Random Forest because of its better behaviour. The error of RF deceases rapidly and becomes stable as the number of trees increases into the forest.

The Neural Network did not overfit but it gave the worst prediction; e.g., in predicting the Corg the MSE (mean squared error) during the training was $393*10^6$ vs. $62*10^6$ for SVM and $85*10^6$ for RF. The MSE during the test step was $402*10^6$ vs. $77*10^6$ for SVM and $63*10^6$ for RF. Consequently we decided to use the Random Forest to create a metamodel of DNDC-EU. RF will be useful also during the variables' importance assessment. The SVM performance was quite similar to the RF one, with a higher validation MSE.

4.4 Integration of RF metamodel into CCAT

To assess the impact of Cross Compliance measures on air, water and soil attributes a simulation platform, which integrates several models, have been developed. This tool (Cross Compliance Assessment Tool) allows studying the changes in previously selected environmental indicators (outputs), according to a specified scenario (inputs). The DNDC-EU metamodels represent only a part of this platform and it is used to estimate the N2O emission, the N leached, the N surplus across the EU agricultural lands (Fig 8).

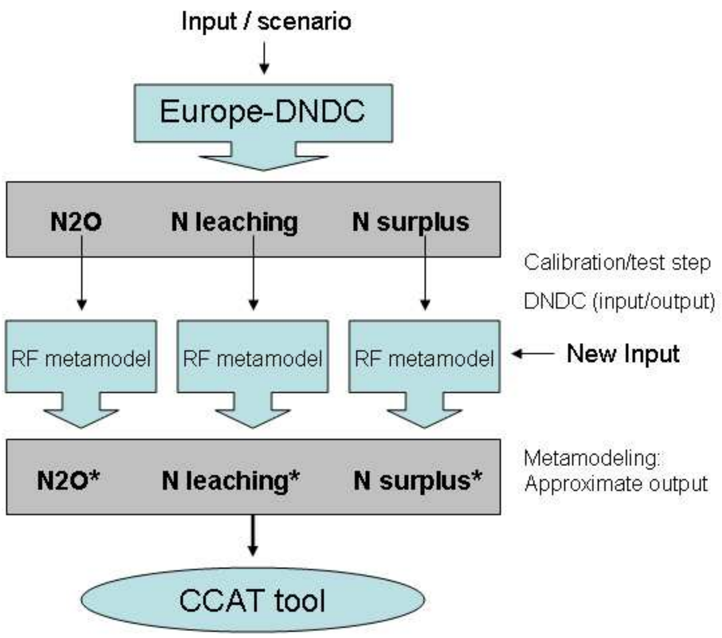

Figure 10: Metamodeling approach into CCAT

At the beginning the simulations through Europe-DNDC have been carried out at HSMU level. The selected subsample included about 20000 HSMU among the whole EU25 data set. The results have been displayed with this detailed resolution.

Afterward we had to upscale to CCAT-NUTS level to integrate our metamodel into the final platform.

The aggregation of HSMU values have been carried out by means of a *weighted area algorithm* taking into account both the input and output data on the whole NUTS agricultural land covered by the studied crops. Care must be taken, as frequencies distributions, dispersions and spatial correlations for the same variable change when the data support size changes [Chiles and Delfiner, 1999].

At last, our Random Forests have been calibrated and validated on the NUTS level. The quality and the accuracy of these steps are lower than by using HSMU resolution; the RF performance will be reduced because of the coarser information and the small numbers of samples (Tab 2).

Table 2: Metamodels' performance during the train and test steps for each scenario and environmental indicators.

metamodel	Train MSE	Train %var explained	Test MSE	Test %var explained
S1				
RF-N2O	3.58	61.55	3.14	74.52
RF-Nleaching	958.94	67.98	533.52	83.4
RF-Nsurplus	734	89.84	685.53	91.55
S2				
RF-N2O	2.40	67.36	1.56	82.2
RF-Nleaching	900.03	59.9	423.3	81.03
RF-Nsurplus	802.63	91.58	832.36	91.28
S3				
RF-N2O	1.80	70.6	2.38	65.3
RF-Nleaching	612.58	69.02	484.25	74.71
RF-Nsurplus	706.1	69.03	675.98	74.47
S4				
RF-N2O	2.17	66.51	1.6	61.49
RF-Nleaching	862.1	67.12	876.9	52.05
RF-Nsurplus	1040	54.88	796.8	54.03
S5				
RF-N2O	3.99	61.87	5.8	58.15
RF-Nleaching	1544	66	1389	72.19
RF-Nsurplus	1940	14.33	3142	27.93
S6				
RF-N2O	6.3	30.56	4.55	21.6
RF-Nleaching	1308	57.58	1000	58
RF-Nsurplus	506.22	64.37	970	44.7
S7				
RF-N2O	7.3	44.8	6.5	58.7
RF-Nleaching	2730	60	1021	85.65
RF-Nsurplus	426	37	674	36

For one specific scenario we created a Random Forest to predict each environmental indicator (Fig.). Once trained and tested, the forest stores all parameters to be used in the next predictive step, with a new input. Only this tool (predictive RF with all scenario parameters) is integrated into CCAT.

The entire methodology can be resumed as follows:

- ✓ **Import data** on R computing environment: from file.txt (CVS, header + row labels) to file.Rdata
- ✓ Create a **train-test subset**: we randomly select 80% of (input,output) couples for calibration and 20% for validation
- ✓ Create a **Random Forest**: we use the *randomForest* package in R to train and validate the model. All the forest parameters for a specific scenario and for each indicator are stored to be used in the predictive phase with a new input.
- ✓ **Sensitivity analysis**: by means of *forest$Importance* function we are able to point out the importance of each variable in estimating one indicator (see Annex 2). This analysis is based on the *mean decrease accuracy* criterion [Breiman, 2001].
- ✓ **Integration into CCAT**: the model, calibrated and validated, is included into the simulation platform. It's able to estimate the studied indicators with a new input, according to a specific scenario and implementation rate.

The R scripts are attached in the final appendix; they can be run both in R-GUI mode or batch mode. The details of calibration and validation steps are also attached as appendix.

4.5 List of predictors used for metamodeling

From the original Europe-DNDC input files (Fig 1) we screened out the less important predictors to estimate the selected indicators. At last we selected the following predictors (Tab 3 & 4) to feed the RF metamodels:

Table 3: Main corn - predictors' attributes

Predictor	Mean	Standard deviation	Minimum	Maximum
N Fertilizer rate (kg ha^{-1} y^{-1})	56.58	46.6	0	232.2
N in manure (kg ha^{-1} y^{-1})	124.6	100.14	0	311.63
N deposition (kg ha^{-1} y^{-1})	66	26.42	5.17	130.43
N fixation (kg ha^{-1} y^{-1})	3.5	5.45	0	47.47
N in root residue (kg ha^{-1} y^{-1})	33.8	14.69	0	77.16
Soil Bulk density (g cm^{-3})	1.003	0.39	0.13	1.83
Soil Organic Carbon in topsoil (mass fraction)	0.027	0.014	0.0058	0.09
Soil pH (in topsoil)	7.49	0.59	5.42	8.39
Soil clay content (fraction)	0.25	0.057	0.09	0.47
Annual precipitation (mm y^{-1})	791	247.9	200	1854
Yearly Mean Maximum temperature (^{o}C)	15.2	3.05	6.58	22.80
Yearly Mean Minimum temperature (^{o}C)	6.47	2.63	-0.45	14.28

Table 4: Main barley - predictors' attributes

Predictor	Mean	Standard deviation	Minimum	Maximum
N Fertilizer rate (kg ha^{-1} y^{-1})	58.50	63.83	2.02	390.6
N in manure (kg ha^{-1} y^{-1})	15.21	31.95	0	189.67
N deposition (kg ha^{-1} y^{-1})	58.51	37.38	0.63	311.85
N fixation (kg ha^{-1} y^{-1})	0.5	0.67	0	4.34
N in root residue (kg ha^{-1} y^{-1})	29.89	33.64	0.29	386.41
Soil Bulk density (g cm^{-3})	0.9	0.41	0.14	1.86
Soil Organic Carbon in topsoil (mass fraction)	0.028	0.023	0.0066	0.15
Soil pH (in topsoil)	7.47	0.6	5.42	8.39
Soil clay content (fraction)	0.26	0.054	0.09	0.55
Annual precipitation (mm y^{-1})	764	246.7	256	1888
Yearly Mean Maximum temperature (^{o}C)	15	3.28	5.14	22.76
Yearly Mean Minimum temperature (^{o}C)	6.17	2.97	-3.9	14.87

For each scenario we carried out a sensibility analysis based on the *forest$importance* function included into our RF metamodel. The evaluation of the predictors' importance is based on the *mean decrease accuracy* criterion, which is described by two indexes: the mean square error and the node impurity [Breiman, 2001]. The RF algorithm computes the importance of a predictor variable by looking at how much prediction error increase when the out-of-bag data for that variable is permuted while all others are left unchanged [Liaw et al, 2002]. The bigger this loss is, the most important the predictor is to estimate the indicator (see Annex 2).

5 Conclusion

The introduction of direct payments for environmental services needs the implementation of assessment tools to quantify the real impact of these conservative measures. The possible payoffs can include, e.g., the soil protection from wind and water runoff, the air and water quality enhancement, the soil organic matter recovery, the conservation of natural habitats and biodiversity. The cons could be represented, e.g., by the additional costs for adapting to more sustainable practices and for a starting reduction of yield.

The CCAT project aims to develop an integrated simulation platform for a quantitative assessment of Cross-Compliance measures across the EU25 agricultural milieu by means of environmental indicators.

The CAPRI/Europe-DNDC modeling approach focuses on the estimation of N2O emission, N leaching and surplus.

We designed a series of scenarios by varying three alternative management practices, namely no-till, max manure amendment and catch crop, for a corn monoculture on a representative HSMU EU25 subset. We pointed out that the no-tillage scenario reduces both the N2O emission (-20%) and N leaching (-13%), but increases the N surplus (+6%). Our simulations output suggested that by limiting the manure spreading to 170 kg/ha a year, we can have an environmental benefit in terms of N2O (-24%), N leaching (-14%) and N surplus (-15%) reduction. The last scenario's results indicated that, when the farming system includes a rotation between a productive crop (corn) and a cover crop (alfalfa), these environmental benefits are more marked, comparing with the two previous conservative management scenarios (-27% for N2O, -20% for N leaching and -34% for N surplus).

We have also designed two scenarios for barley monoculture (winter crop) namely no-till and max manure. In this case we have not observed significant differences between the reference scenario and the alternative management practices. By implementing no-tillage we pointed out a slight reduction in N2O emission (-4%) and N leaching (-2.45%), while the N surplus remained almost unchanged. The max manure scenario resulted in a very small decrease in N2O (-1.7%) and N surplus (-3%); the N leaching did not significantly change.

The metamodels have been developed to reduce the running time and memory consumption of the original complex DNDC code, and to highlight the input/output relationships. After a preliminary comparison between some metamodeling methods, we selected the Random-Forest one (RF) due to its better performance and because it is very user-friendly and easily parallelized. Moreover it provides useful information about the estimate of error and the variable importance (sensibility analysis). Different RF have been trained and tested for each indicator at NUTS level, according to the selected CC scenarios. The optimal predictive Random Forests will be integrated into CCAT tool to estimate the N2O emission, N leaching and surplus on the basis of new inputs.

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Annex 1:

Random Forest calibration at NUTS level (DNDC vs. RF Metamodel output values)

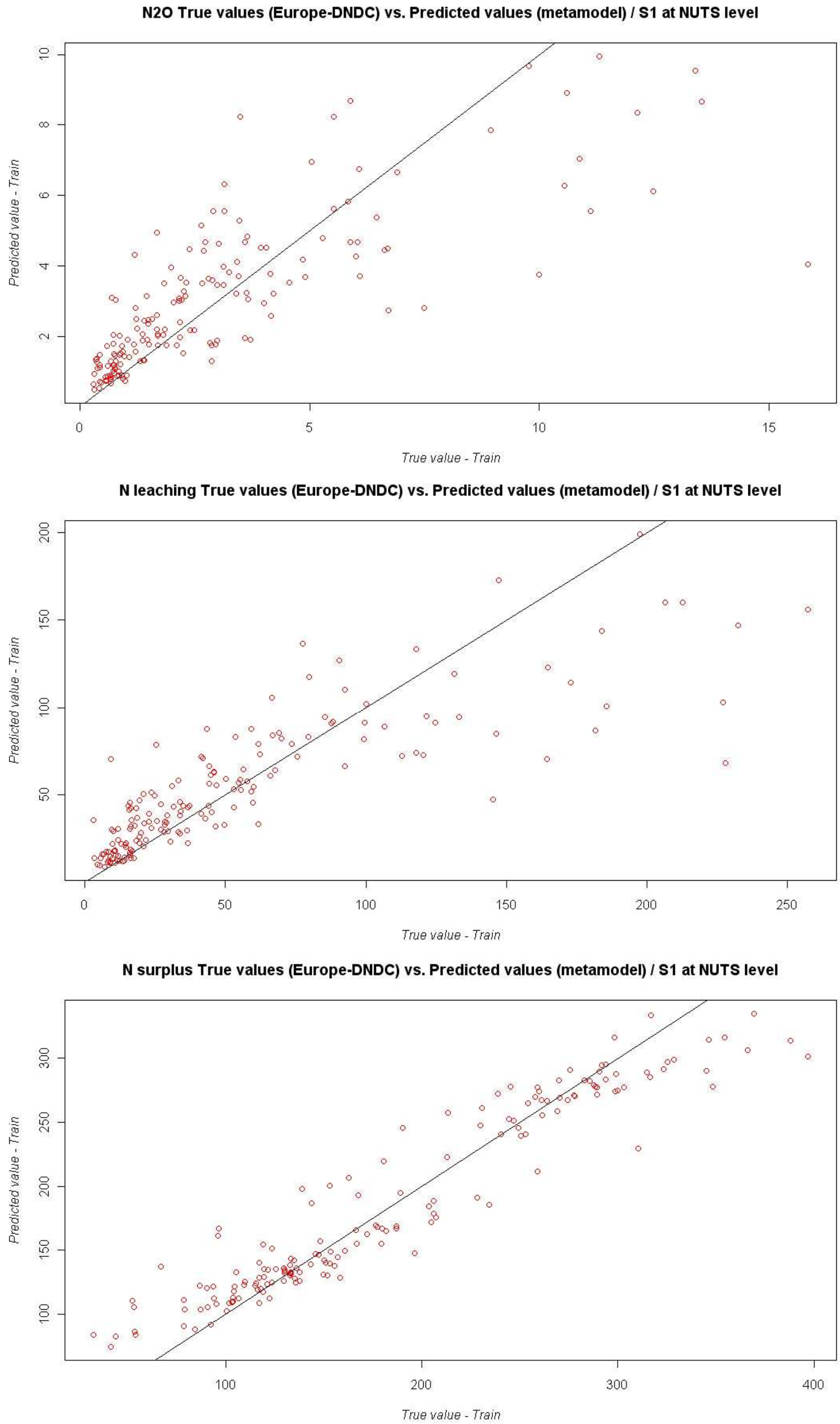

Figure 11: S1 calibration scattergram. DNDC (true values) vs. metamodel values by the RF metamodel at NUTS level.

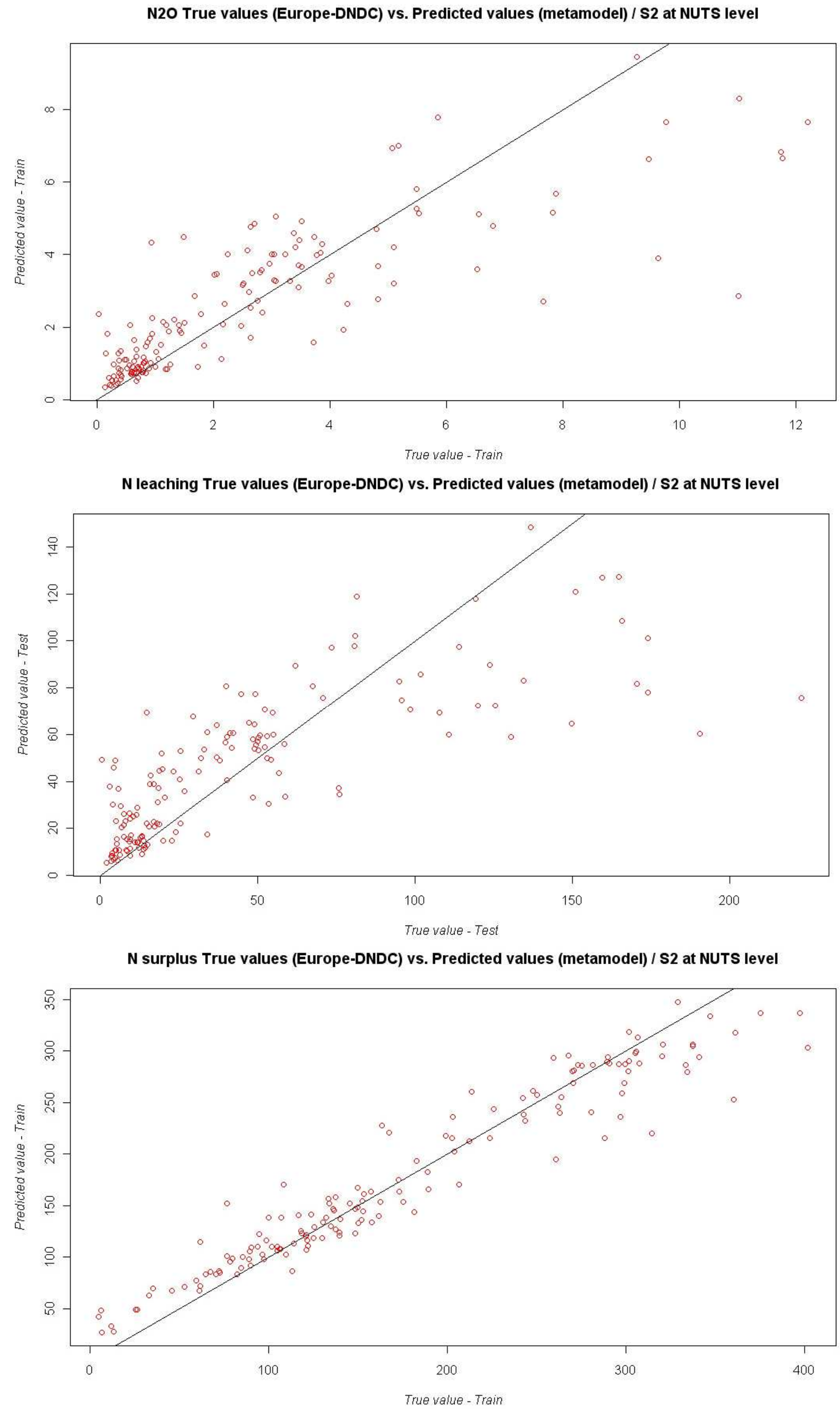

Figure 12: S2 calibration scattergram. DNDC (true values) vs. predicted values by RF metamodel at NUTS level.

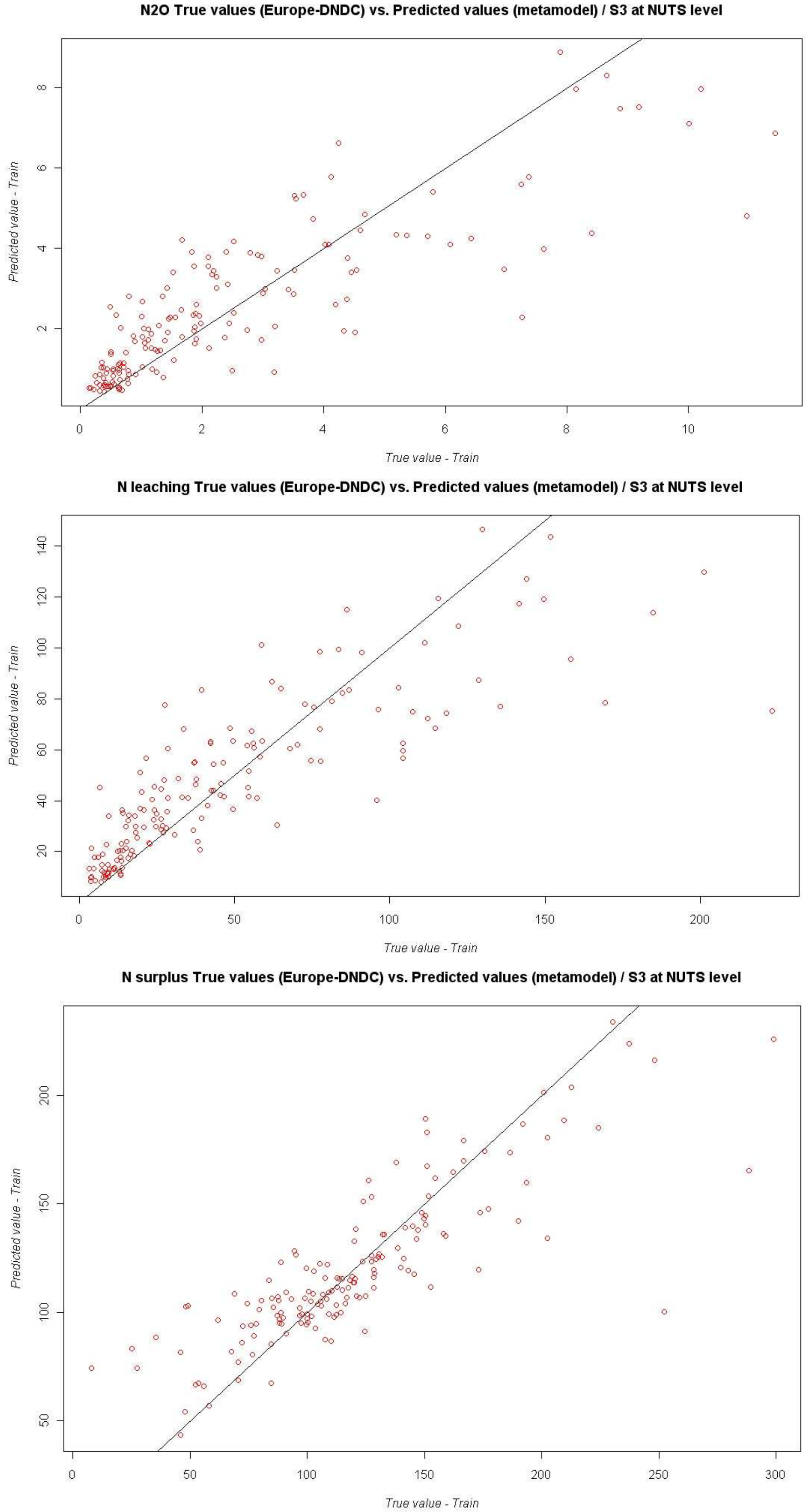

Figure 13: S3 calibration scattergram. DNDC (true values) vs. predicted values by RF metamodel at NUTS level.

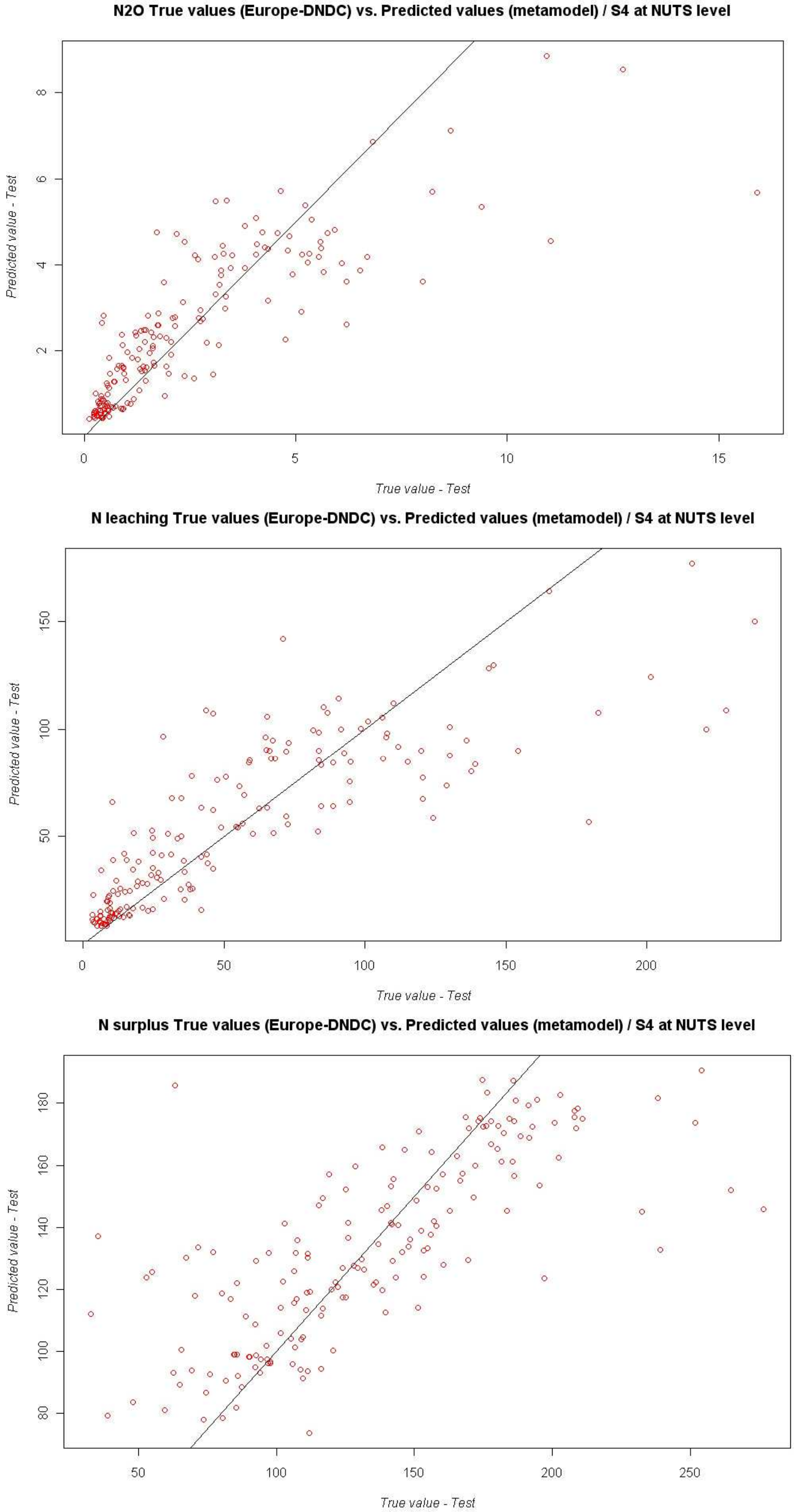

Figure 14: S4 calibration scattergram. DNDC (true values) vs. predicted values by RF metamodel at NUTS level.

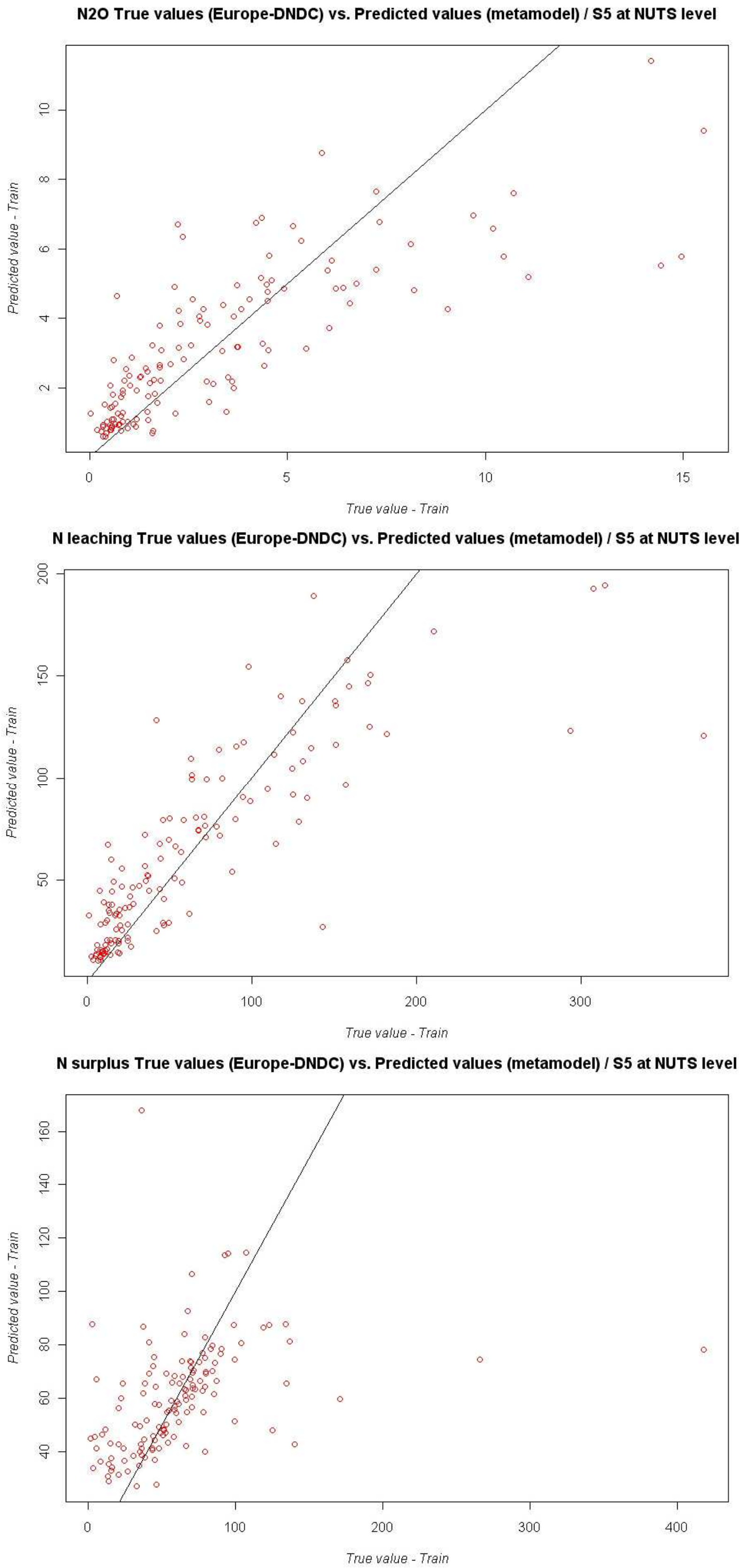

Figure 15: S5 calibration scattergram. DNDC (true values) vs. predicted values by RF metamodel at NUTS level.

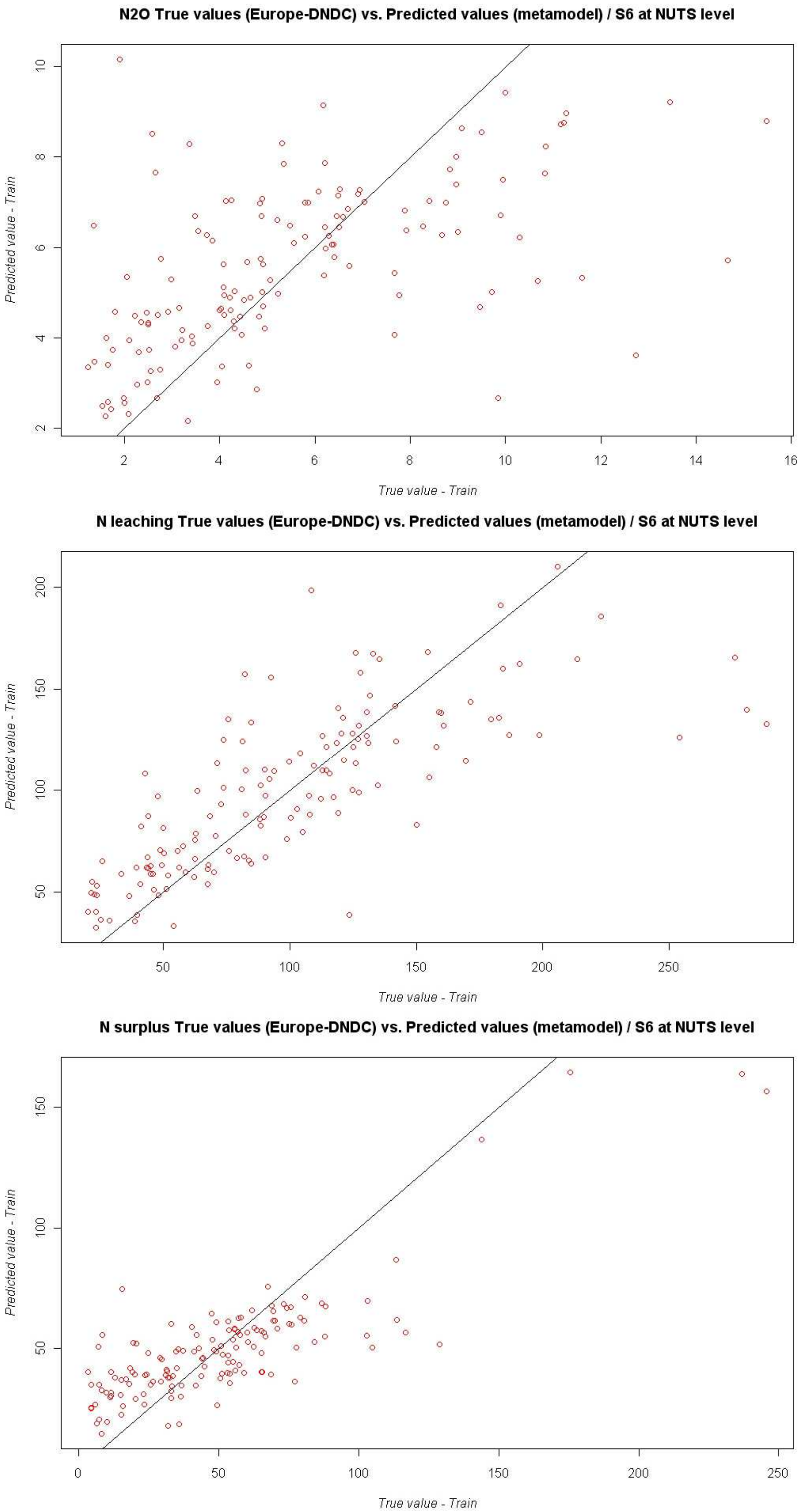

Figure 16: S6 calibration scattergram. DNDC (true values) vs. predicted values by RF metamodel at NUTS level.

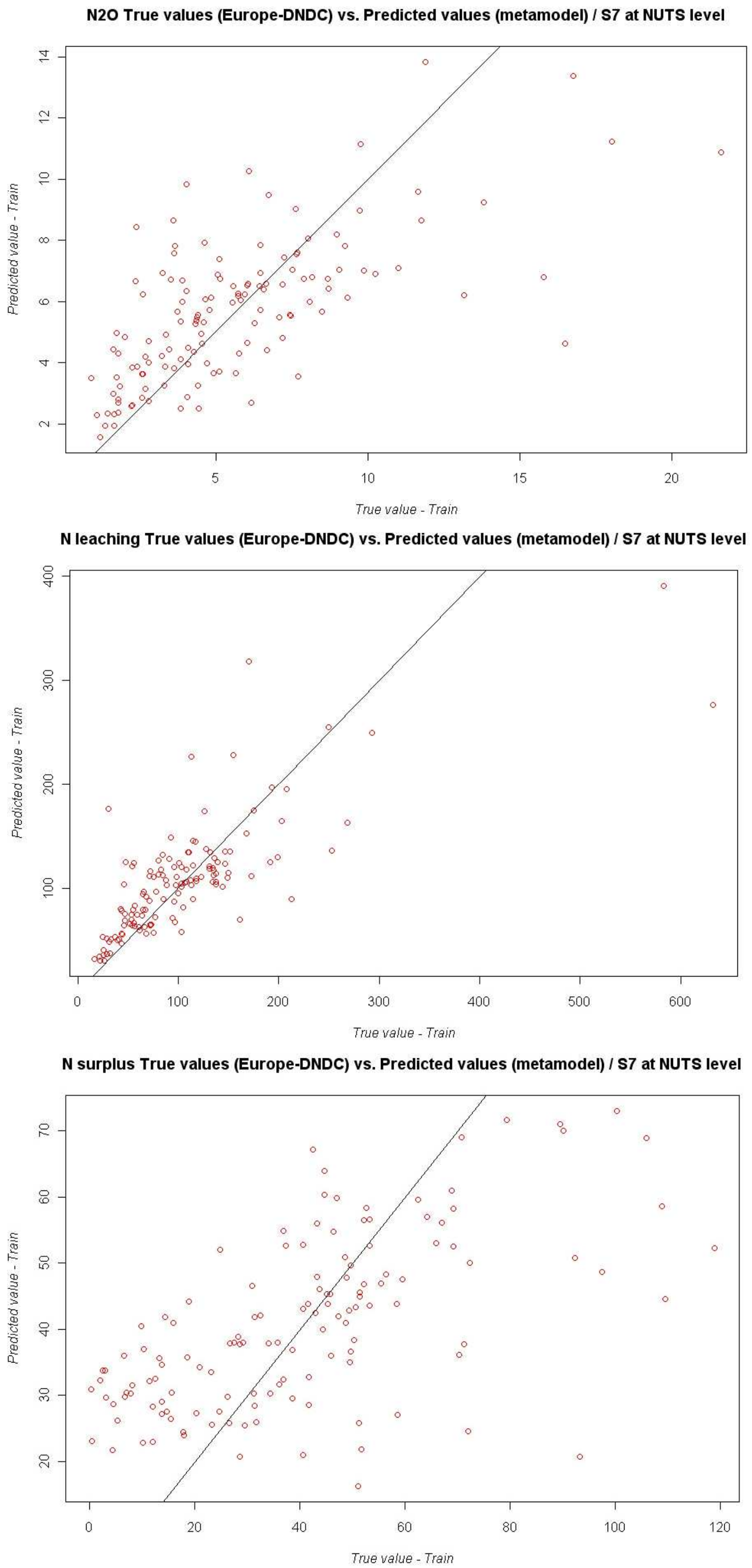

Figure 17: S7 calibration scattergram. DNDC (true values) vs. predicted values by RF metamodel at NUTS level.

Annex 2:

Sensitivity analysis – predictors' importance assessment by means of RF mean decrease accuracy (node purity)

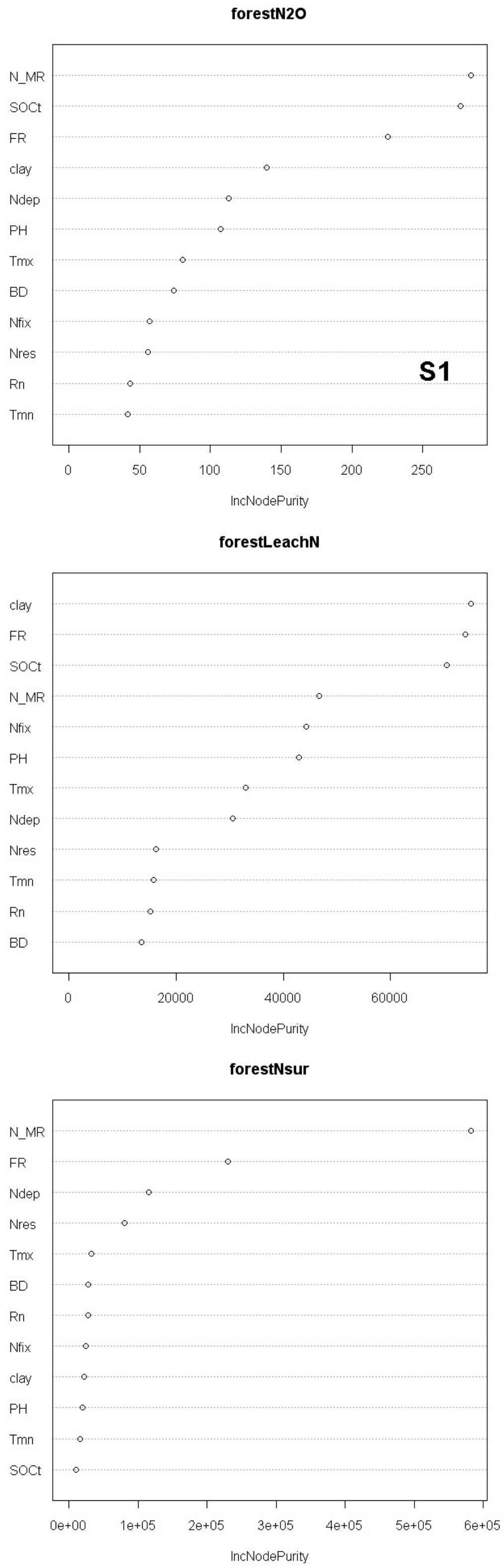

Figure 18: S1 predictors' importance graphical representation (node purity calculated by means of RF and based on mean decrease accuracy criterion)

Table 5: S1 numerical values of predictors' importance. Underlined the most important variables for estimating the environmental indicators.

Predictor-**S1**	N surplus	N leaching	N_2O emissions
N Fertilizer rate (kg ha^{-1} y^{-1})	<u>230446 (2)</u>	<u>73959 (2)</u>	<u>225 (3)</u>
N in manure (kg ha^{-1} y^{-1})	<u>582333 (1)</u>	46676 (4)	<u>284 (1)</u>
N deposition (kg ha^{-1} y^{-1})	<u>115668 (3)</u>	30531 (8)	113 (5)
N fixation (kg ha^{-1} y^{-1})	24645 (8)	44358 (5)	56 (9)
N in root residue (kg ha^{-1} y^{-1})	80288 (4)	16186 (9)	55 (10)
Soil Bulk density (g cm^{-3})	28254 (6)	13448 (12)	74 (8)
Soil Organic Carbon in topsoil (mass fraction)	9908 (12)	<u>70477 (3)</u>	<u>276 (2)</u>
Soil pH (in topsoil)	19065 (10)	42997 (6)	107 (6)
Soil clay content (fraction)	21942 (9)	<u>75086 (1)</u>	139 (4)
Annual precipitation (mm y^{-1})	27968 (7)	15222 (11)	42 (11)
Yearly Mean Maximum temperature (^oC)	31798 (5)	33014 (7)	80 (7)
Yearly Mean Minimum temperature (^oC)	16262 (11)	15831 (10)	41 (12)

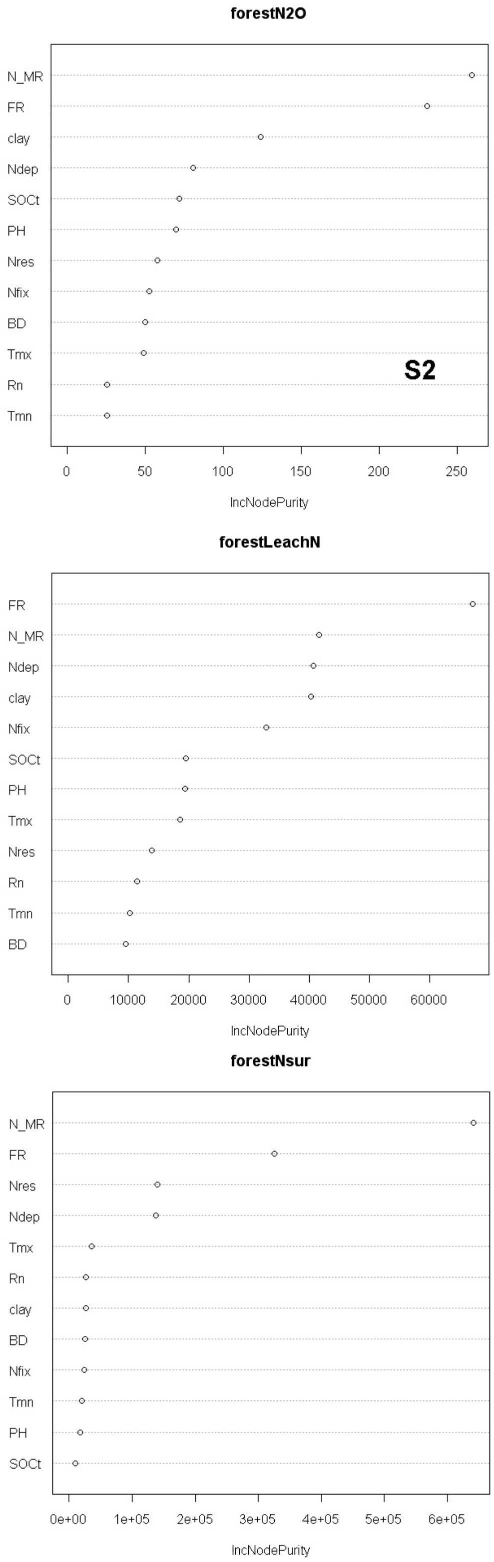

Figure 19: S2 predictors' importance graphical representation (node purity calculated by means of RF and based on mean decrease accuracy criterion)

Table 6: S2 numerical values of predictors' importance. Underlined the most important variables for estimating the environmental indicators.

Predictor-**S2**	N surplus	N leaching	N_2O emissions
N Fertilizer rate (kg ha^{-1} y^{-1})	<u>325557 (2)</u>	<u>67185 (1)</u>	<u>230 (2)</u>
N in manure (kg ha^{-1} y^{-1})	<u>641389 (1)</u>	<u>41605 (2)</u>	<u>259 (1)</u>
N deposition (kg ha^{-1} y^{-1})	136924 (4)	<u>40693 (3)</u>	80 (4)
N fixation (kg ha^{-1} y^{-1})	23425 (9)	32934 (5)	52 (8)
N in root residue (kg ha^{-1} y^{-1})	<u>140181 (3)</u>	13870 (9)	57 (7)
Soil Bulk density (g cm^{-3})	25391 (8)	9514 (12)	50 (9)
Soil Organic Carbon in topsoil (mass fraction)	9346 (12)	19538 (6)	71 (5)
Soil pH (in topsoil)	17915 (11)	19392 (7)	69 (6)
Soil clay content (fraction)	26040 (7)	<u>40358 (4)</u>	<u>123 (3)</u>
Annual precipitation (mm y^{-1})	27255 (6)	11418 (10)	25 (11)
Yearly Mean Maximum temperature (^{o}C)	35036 (5)	18621 (8)	48 (10)
Yearly Mean Minimum temperature (^{o}C)	19720 (10)	10171 (11)	25 (12)

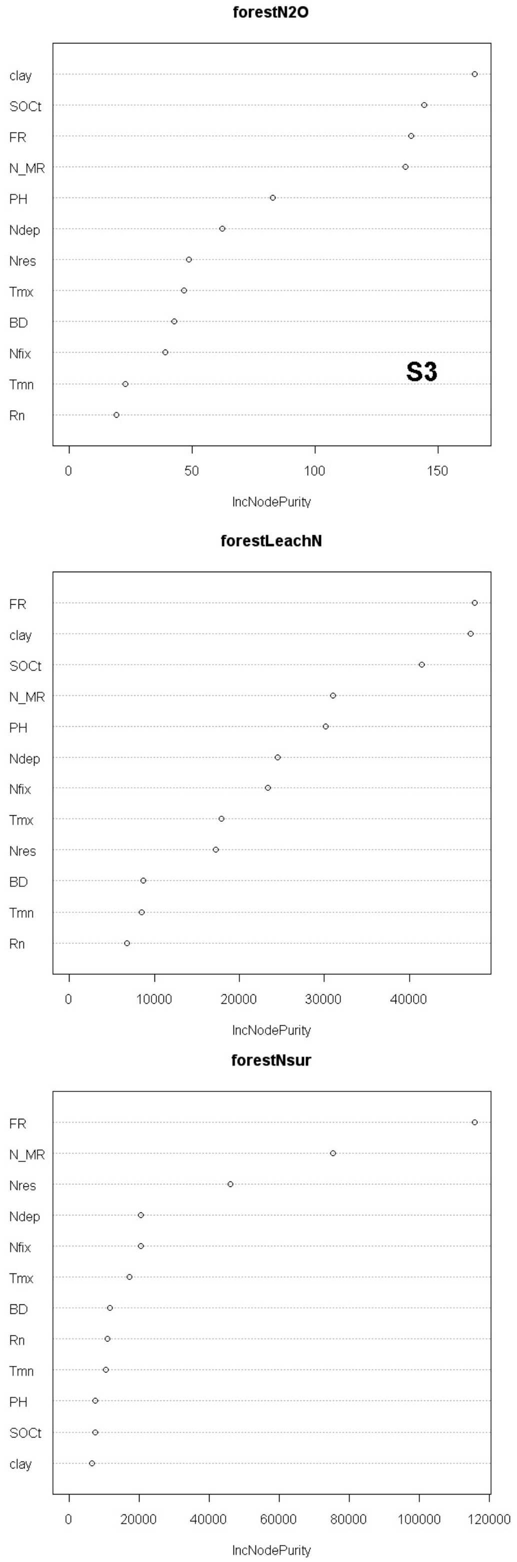

Figure 20: S3 predictors' importance graphical representation (node purity calculated by means of RF and based on mean decrease accuracy criterion)

Table 7: S3 numerical values of predictors' importance. Underlined the most important variables for estimating the environmental indicators.

Predictor-**S3**	N surplus	N leaching	N_2O emissions
N Fertilizer rate (kg ha^{-1} y^{-1})	<u>115972 (1)</u>	<u>47721 (1)</u>	<u>139 (3)</u>
N in manure (kg ha^{-1} y^{-1})	<u>75415 (2)</u>	30978 (4)	<u>136 (4)</u>
N deposition (kg ha^{-1} y^{-1})	20454 (4)	24485 (6)	62 (6)
N fixation (kg ha^{-1} y^{-1})	20391 (5)	23339 (7)	39 (10)
N in root residue (kg ha^{-1} y^{-1})	<u>46131 (3)</u>	17232 (9)	48 (7)
Soil Bulk density (g cm^{-3})	11457 (7)	8710 (10)	42 (9)
Soil Organic Carbon in topsoil (mass fraction)	7284 (11)	<u>41429 (3)</u>	<u>144 (2)</u>
Soil pH (in topsoil)	7408 (10)	30128 (5)	82 (5)
Soil clay content (fraction)	6442 (12)	<u>47236 (2)</u>	<u>165 (1)</u>
Annual precipitation (mm y^{-1})	10957 (8)	6772 (12)	19 (12)
Yearly Mean Maximum temperature (^{o}C)	17165 (6)	17871 (8)	46 (8)
Yearly Mean Minimum temperature (^{o}C)	10432 (9)	8516 (11)	22 (11)

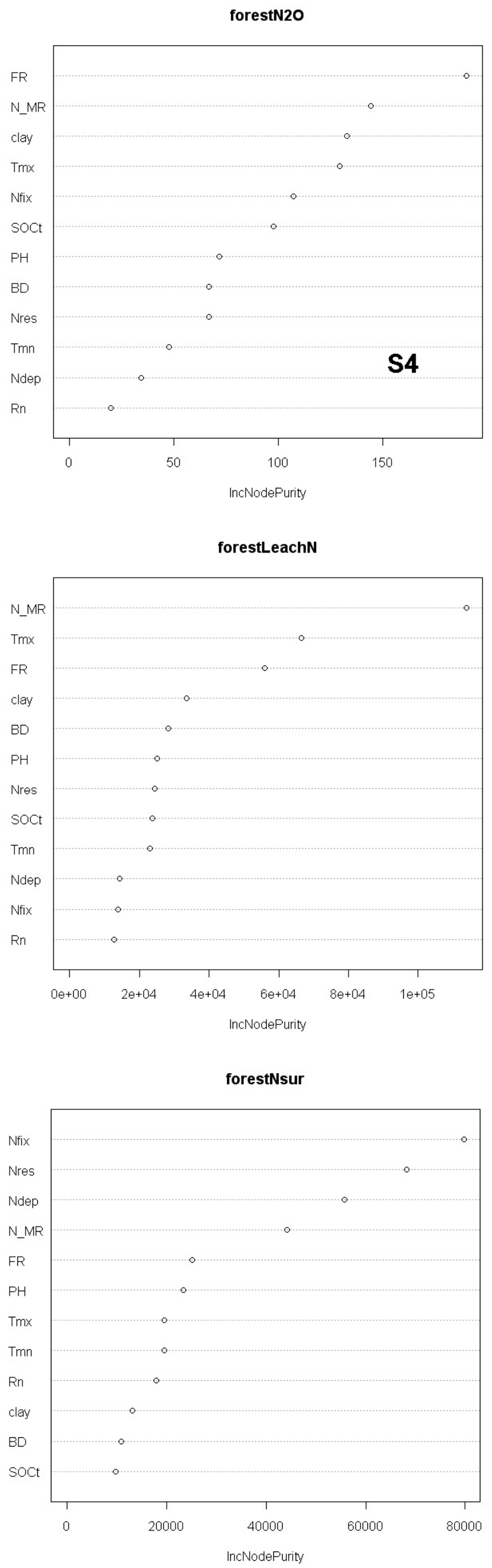

Figure 21: S4 predictors' importance graphical representation (node purity calculated by means of RF and based on mean decrease accuracy criterion)

Table 8: S4 numerical values of predictors' importance. Underlined the most important variables for estimating the environmental indicators.

Predictor-**S4**	N surplus	N leaching	N_2O emissions
N Fertilizer rate (kg ha^{-1} y^{-1})	25051 (5)	<u>55876 (3)</u>	<u>190 (1)</u>
N in manure (kg ha^{-1} y^{-1})	44182 (4)	<u>113905 (1)</u>	<u>144 (2)</u>
N deposition (kg ha^{-1} y^{-1})	<u>55804 (3)</u>	14385 (10)	34 (11)
N fixation (kg ha^{-1} y^{-1})	<u>79833 (1)</u>	13845 (11)	107 (5)
N in root residue (kg ha^{-1} y^{-1})	<u>68309 (2)</u>	24401 (7)	66 (9)
Soil Bulk density (g cm^{-3})	10851 (11)	28184 (5)	66 (8)
Soil Organic Carbon in topsoil (mass fraction)	9688 (12)	23609 (8)	97 (6)
Soil pH (in topsoil)	23303 (6)	25117 (6)	71 (7)
Soil clay content (fraction)	13060 (10)	33648 (4)	<u>132 (3)</u>
Annual precipitation (mm y^{-1})	17846 (9)	12623 (12)	19 (12)
Yearly Mean Maximum temperature (^oC)	19525 (7)	<u>66535 (2)</u>	<u>129 (4)</u>
Yearly Mean Minimum temperature (^oC)	19428 (8)	23061 (9)	47 (10)

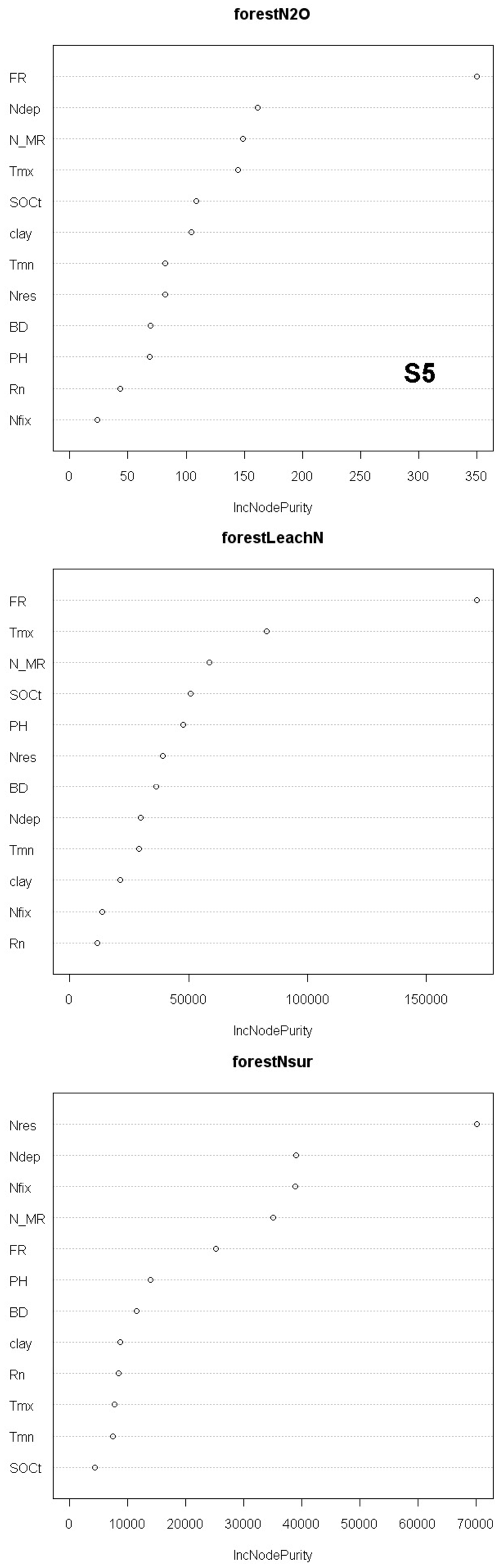

Figure 22: S5 predictors' importance graphical representation (node purity calculated by means of RF and based on mean decrease accuracy criterion)

Table 9: S5 numerical values of predictors' importance. Underlined the most important variables for estimating the environmental indicators.

Predictor-**S5**	N surplus	N leaching	N_2O emissions
N Fertilizer rate (kg ha^{-1} y^{-1})	25206 (5)	171341 (1)	349 (1)
N in manure (kg ha^{-1} y^{-1})	35075 (4)	58608 (3)	149 (3)
N deposition (kg ha^{-1} y^{-1})	38990 (2)	29706 (8)	161 (2)
N fixation (kg ha^{-1} y^{-1})	38916 (3)	13628 (11)	23(12)
N in root residue (kg ha^{-1} y^{-1})	70210 (1)	38974 (6)	81 (8)
Soil Bulk density (g cm^{-3})	11460 (7)	36229 (7)	69 (9)
Soil Organic Carbon in topsoil (mass fraction)	4335 (12)	50873 (4)	108 (5)
Soil pH (in topsoil)	13901(6)	47808 (5)	68 (10)
Soil clay content (fraction)	8736 (8)	21121 (10)	104 (6)
Annual precipitation (mm y^{-1})	8431 (9)	11472 (12)	43 (11)
Yearly Mean Maximum temperature (^{o}C)	7765 (10)	82952(2)	144 (4)
Yearly Mean Minimum temperature (^{o}C)	7366 (11)	29163 (9)	81 (7)

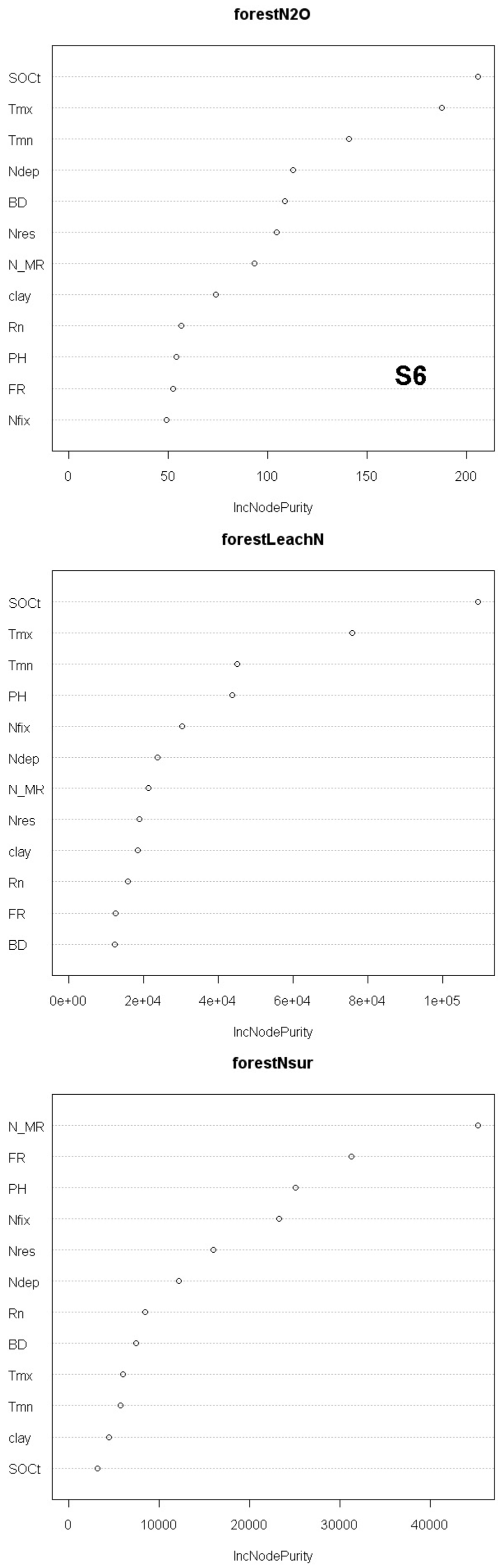

Figure 23: S6 predictors' importance graphical representation (node purity calculated by means of RF and based on mean decrease accuracy criterion)

Table 10: S6 numerical values of predictors' importance. Underlined the most important variables for estimating the environmental indicators.

Predictor-**S6**	N surplus	N leaching	N_2O emissions
N Fertilizer rate (kg ha^{-1} y^{-1})	<u>31230 (2)</u>	12362 (11)	52 (11)
N in manure (kg ha^{-1} y^{-1})	<u>45299 (1)</u>	21133 (7)	93 (7)
N deposition (kg ha^{-1} y^{-1})	12166 (6)	23699 (6)	112 (4)
N fixation (kg ha^{-1} y^{-1})	<u>23215 (4)</u>	30280 (5)	49 (12)
N in root residue (kg ha^{-1} y^{-1})	15992 (5)	18805 (8)	104 (6)
Soil Bulk density (g cm^{-3})	7443 (8)	12331 (12)	108 (5)
Soil Organic Carbon in topsoil (mass fraction)	3195 (12)	<u>109416 (1)</u>	<u>205 (1)</u>
Soil pH (in topsoil)	<u>25051 (3)</u>	43629 (4)	54 (10)
Soil clay content (fraction)	4445 (11)	18493 (9)	74 (8)
Annual precipitation (mm y^{-1})	8416 (7)	15856 (10)	56.44 (9)
Yearly Mean Maximum temperature (^oC)	6008 (9)	<u>75774 (2)</u>	<u>187 (2)</u>
Yearly Mean Minimum temperature (^oC)	5709 (10)	<u>44914 (3)</u>	<u>141 (3)</u>

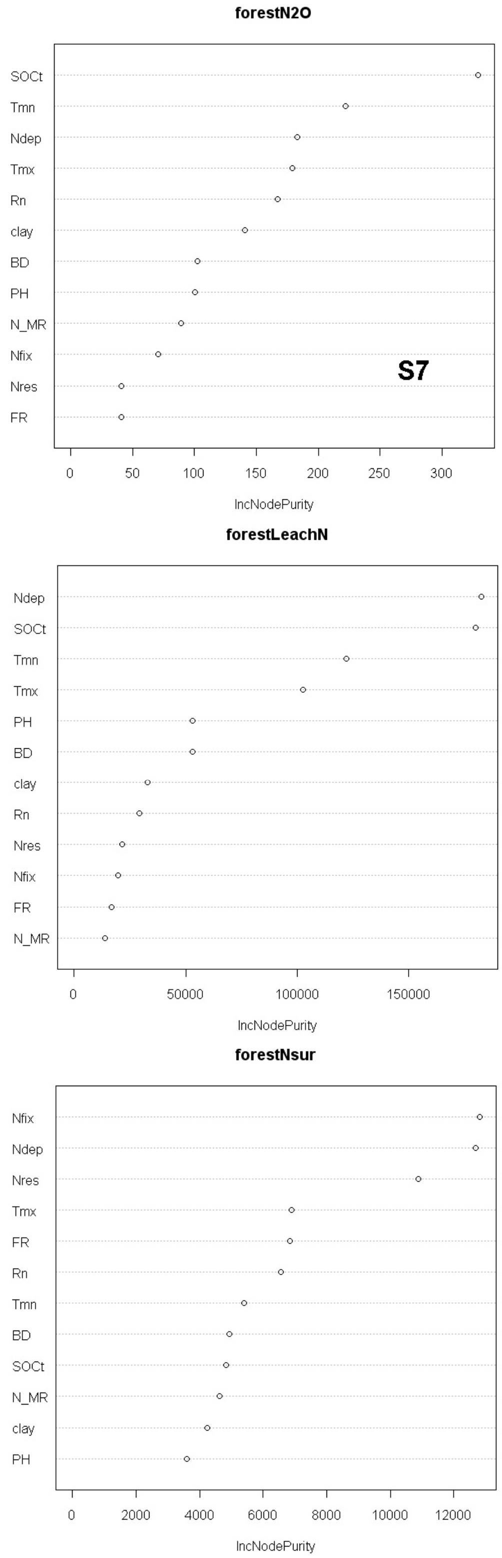

Figure 24: S7 predictors' importance graphical representation (node purity calculated by means of RF and based on mean decrease accuracy criterion)

Table 11: S7 numerical values of predictors' importance. Underlined the most important variables for estimating the environmental indicators.

Predictor-**S7**	N surplus	N leaching	N_2O emissions
N Fertilizer rate (kg ha^{-1} y^{-1})	6850 (5)	16635 (11)	40 (12)
N in manure (kg ha^{-1} y^{-1})	4639 (10)	13792 (12)	89 (9)
N deposition (kg ha^{-1} y^{-1})	<u>12689 (2)</u>	<u>182678 (1)</u>	<u>182 (3)</u>
N fixation (kg ha^{-1} y^{-1})	<u>12822 (1)</u>	19612 (10)	70 (10)
N in root residue (kg ha^{-1} y^{-1})	<u>10881 (3)</u>	21445 (9)	104 (6)
Soil Bulk density (g cm^{-3})	4939 (8)	53104 (6)	102 (7)
Soil Organic Carbon in topsoil (mass fraction)	4833 (9)	<u>180120 (2)</u>	<u>329 (1)</u>
Soil pH (in topsoil)	3590 (12)	53215 (5)	100 (8)
Soil clay content (fraction)	4228 (11)	3306 (7)	140 (6)
Annual precipitation (mm y^{-1})	6549 (6)	29359 (8)	167 (6)
Yearly Mean Maximum temperature (^oC)	6885 (4)	102729(4)	179 (4)
Yearly Mean Minimum temperature (^oC)	5398 (7)	<u>121939 (3)</u>	<u>222 (2)</u>