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Approach for Uncertainty Quantification (UQ) of INTEGRATOR at the European scale

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1 Background of this internal note

This documentation is part of Deliverable 6.3.4 in WP 6.3: Uncertainty of European N & GHG emissions. Deliverable 6.3.4 is a progress report on preparation for UQ for the three sources of information: (i) results from bottom-up GIS modelling (ii) estimates based on independent measurements, (iii) results from top-down inverse modelling. This documentation describes the plans for C5, limited to the *INTEGRATOR prototyp*e model. The key uncertainties described are related to input data (except the 'uncertainty' in a scenario) and parameters. However, the uncertainties due to model structure will also be dealt with by comparing results of the INTEGRATOR prototype with those of detailed ecosystem models. The ideas with respect to detailed ecosystem models are mentioned, but these have to be worked out further at the next C5/C6 meeting in October 22-23 2008. Furthermore, the ideas with respect to a second UQ with the final INTEGRATOR model are mentioned.

2 General approach

An uncertainty analysis will be carried out with the INTEGRATOR prototype for EU27+3, applied to all NCUs, focusing on the period 1970-2030. The INTEGRATOR prototype consists of (i) MITERRA, (ii) EFISCEN, (iii) YASSO and (iv) empirical relationships between GHG emissions and site characteristics and/or soil properties. The aim is to analyse how uncertainties in model inputs and parameters propagate to model outputs, using Monte Carlo analysis, focusing on uncertainties in continuous model inputs (e.g. soil properties) and model parameters (e.g. biomass expansion factors excretion factors and emission fractions), while neglecting uncertainties in scenario related model inputs (climate, animal numbers, land cover etc) and in categorical data (e.g. soil type, drainage status). The approach follows the "Operational methodology for spatial uncertainty quantification and spatial uncertainty analysis of regional scale NEU models" by Heuvelink et al (2008).

Preparations for uncertainty quantification with INTEGRATOR included (see Heuvelink et al., 2008):

Step 1 Assessment of the boundaries of the modelled system, its inputs and outputs
Step 2 Selection of the model output(s) for which the uncertainty must be assessed
Step 3 Define the uncertainty sources that are included in the analysis
Step 4 Assignment of uncertainties (probability distributions) in soil properties and model inputs (and parameters) at NCU level

3 Assessment of the boundaries of the modelled system, its inputs and outputs

Regarding the boundaries of the modelled system by INTEGRATOR, the following decision were made:

- *Spatial extent and spatial resolution*. INTEGRATOR will be applied for EU 27+3 countries using a schematization based on so-called NitroEurope Computational Units (NCU's), being spatial explicit units with homogeneous characteristics. The size of the NCUs is highly variable: mean area = 163 km^2, SD = 557 km^2NCU's are in fact HSMUs without CORINE land use. In

HSMUs CORINE 2000 land use is used, for NCUs we will use land use scenarios from CLUE. One NCU can have multiple land use scenarios. The implicit assumption of using the NCU as smallest spatial calculation unit is that spatial variability within NCUs is not (explicitly) considered. At NCU level, averages are used with their uncertainty, which includes spatial variability.

- *Vertical extent and resolution*: important is soil depth: this must be defined in view of the assigned soil properties. INTEGRATOR is a one-layer model meaning that vertical extent, resolution and support are the same. The overall soil layer in INTEGRATOR is 1m. The soil properties needed in view of N_2O and NO_x emission (fractions) and N leaching fractions are related to the topsoil (plough layer or upper 30 cm in forest soils). NH_3, CO_2 and CH_4 emissions are not related to soil properties in the INTEGRATOR prototype (only to groundwater level). Regarding carbon and nitrogen accumulation, the idea is to use the one compartment YASSO model (no layering). The present depth considered in YASSO covers the organic layer on top of mineral soil (if present) and a 1 m thick mineral soil layer. We intend to calibrate the model to cover the upper 30 cm, assuming that the amount of organic matter between 30 and 100 cm is inert (to be discussed with Jari Liski).
- *Temporal extent and temporal resolution*. The period 1970-2030 at an annual/ 5 year resolution. The model outputs will be presented for the year 1970, 2000 and 2030.
- *Spatial and/or temporal support of model outputs*. This refers to the spatial area or volume and temporal interval over which the model output is aggregated. It is the average model output over the NCU, aggregated over the complete soil profile and the whole year. Further spatial aggregation to NUTS 2/1 level or entire countries will also be done.

4 Selection of the model output(s) for which the uncertainty must be assessed

INTEGRATOR has multiple outputs whose uncertainties may be different. Moreover, the contribution of individual uncertainty sources to the model output will differ between outputs. The uncertainty analysis identifies those uncertainty sources that have the largest contribution to the output uncertainty. For the UQ with INTEGRATOR, the outputs given in Table 1 are suggested.

We must also define the type of system for which we make the comparisons, i.e.:

Total agriculture

- Housing systems
- Grass land
- Arable land

Total non-agricultural land

- Forests
- Peatlands
- Short vegetations

Table 1: Model outputs of INTEGRATOR (and detailed ecosystem models), for which an Uncertainty Quantification will be made.

Flux	Standard unit
NH_3 emission	kgNH_3-N/ha/year
N_2O emission	kgN_2O-N/ha/year
NO_x emission	kgNO_x-N/ha/year
CH_4 emission	kgCH_4/ha/year
CO_2 emission	kgCO_2/ha/year
C accumulation - Vegetation (trees) - Soil - Total	kgC/ha/year
N budget, i.e - N uptake - N denitrification - N accumulation - N leaching/runoff	kgN/ha/year

5 Uncertainty sources that are included in the analysis

Model output uncertainty is affected by three categories of uncertainty sources: (1) model input uncertainty, (2) model structure uncertainty, and (3) model solution uncertainty. It was concluded that category 3 (model solution uncertainty, which refers to errors caused by rounding, numerical evaluation of integrals, suboptimal optimization solutions etc) has a marginal contribution to the output uncertainty and can therefore be ignored. The uncertainties due to model structure will be dealt with by comparing results of INTEGRATOR with those of detailed ecosystem models. The UQ thus focuses on model input uncertainty, where “inputs”, in accordance with the NEU protocols, are defined as all the bits of information needed to run a model that are not incorporated in the model itself: (1) Initial values (= values of state variables at start of simulation), (2) Model parameters, (3) Environmental constants and variables.

6 Assignment of uncertainties in model inputs

General approach

The uncertainty in model input data will be limited to (i) soil properties and (ii) groundwater levels below peat soils. Uncertainties in categorical data as land use maps and soil maps and in input data such as animal numbers will not be included in the analysis with the INTEGRATOR prototype. Furthermore, we will use the dominant Soil Typological Unit (STU) of each Soil Mapping Unit (SMU) to characterize the soil in an NCU.

Assignment of uncertainties in soil properties

The assignment of uncertainties in soil data and the uncertainties therein for each NCU includes the following data:

- soil physical data: texture, clay, silt and sand content and bulk density,
- soil chemical data: CEC, pH, base saturation, carbon content, nitrogen content, carbonate content

Soil attributes are partly based on the soil map itself (soil texture and soil wetness) but mainly on the SPADE and WISE soil profile databases (clay, silt and sand content, bulk density and soil chemical data). The SPADE and WISE soil profile databases are used to create a soil database with parameter means, ranges, standard deviations and

spatial correlation (to include information on uncertainties) for all soil attributes (see above) per combination of soil type, texture class and aggregated land use type. A spatial allocation is foreseen for all soil properties by (i) relationships with soil, climate zone and land use followed by (ii) kriging and assessing uncertainties in a spatial explicit way. This procedure is described in Reinds et al (in prep.). Later, the (uncertainty range in) assigned soil properties will be compared with national data (e.g. data in the Dutch Soil Information System) to see whether both ranges overlap.
For the INTEGRATOR prototype, not all soil properties mentioned above are relevant. The included soil properties in the UQ are:

- soil physical data: texture
- soil chemical data: pH, carbon content and nitrogen content (C/N ratio).

The soil properties are needed in view of:

- Texture: N_2O and NO_x emission fractions in agricultural soils and N leaching fractions in agricultural soils (classes).
- pH: N_2O and NO_x emission fractions in agricultural soils (classes) and N_2O and NO_x emission relationships in non-agricultural soils (continuous data).
- Carbon content: N leaching fractions in agricultural soils (classes) and N_2O and NO_x emission relationships in non-agricultural soils (continuous data).
- C/N ratio: N immobilization in both agricultural and non-agricultural soils.

NH_3, CO_2 and CH_4 emissions are not related to soil properties in the INTEGRATOR prototype. Furthermore, N_2O and NO_x emission fractions in agricultural soils are only related to classes of for texture, pH and carbon content, implying a low and disjunctive effect of these properties on these emissions. CO_2 and CH_4 emissions from peat soils are only related to groundwater level. For these groundwater level data, a fixed range per land use type will be used.

Assignment of uncertainties in model parameters
The uncertainty in model parameters will include all major parameters in INTEGRATOR, i.e.:
MITERRA

Manure management data

- N and C excretion rates
- Housing fractions
- Fraction of excreted amount stored as liquid manure in the housing system
- Fraction of excreted amount stored in manure storage system

Livestock emission data: NH3, N_2O and NO_x (N2) emission fractions from

- Housing systems,
- Manure storage systems
- Grazing

Manure application data

- Allocation fractions in the manure and N input assessment procedure
- Areas (fractions) of intensively and extensively managed grassland

Nitrogen uptake data

- Yields of intensively and extensively managed grassland (kg dw ha-1)
- Crop yields, being the amount of harvested crop (kg dw ha-1)
- Maximum N content in the harvested crops (kgN.kg dw-1)
- N index (ratio of N amount in crop residues divided by N removed in harvest)
- Uptake fraction(efficiency factor) of the effective N applied (-)
- Ratio between minimum and maximum N uptake (-)
- N input at which the yield does not further respond

Soil emission data:

- NH_3 emission factors from soil systems
- N_2O and NO_x emission fractions from soil systems

Leaching and runoff data

- Runoff fractions
- Leaching fractions from the soil
- Leaching fractions from stored manure

EFISCEN

- Biomass expansion factors
- Yield estimates
- Wood density
- Carbon and nitrogen contents in wood

YASSO

- Decomposition rate constants for fine and coarse woody litter and the various carbon fractions in the soil.

Relationships

- Coefficients in relationships describing CO_2, N_2O and CH_4 exchange rates from soil systems.

7 Remaining aspects in the uncertainty analyses/quantification

Discussion issues remaining in the uncertainty analyses are:

- How to account for spatial correlation in input or parameter uncertainty?
- How to account for correlation in input or parameter uncertainty and the area of NCUs?

The first question is specifically important in view of the spatio-temporal support at which we will produce the target output (NCUs or NUTs2/3 or country or EU27+3 as a whole). If greater than NCU, a post-processing aggregation (upscaling) step is needed. When there is no spatial correlation in input or parameter uncertainty, the uncertainty of the aggregated (upscaled) model output will be much less compared to a situation in which this is included. This aspect still needs further discussion.

8 Uncertainty analyses/quantification with the detailed ecosystem models

For the *detailed ecosystem models*, such as DNDC, Daycent and EPIC, a similar UQ will be carried out, but the number of NCUs (including land use sequences) will be too large to cope with when including an uncertainty analysis. For these models, an UQ will be carried out on selected NCUs , that later on will be aggregated based on similarities in attribute values. Some kind of aggregation of attribute values into fixed or flexible classes is thus required. Detailed models will be applied to e.g. 5-10 NCUs to see whether uncertainty increases with increasing number of NCUs and where it levels off → then apply to Europe (how is still an aspect to be discussed). For one base line year, possibly the application to all NCUs might be possible. A comparison of the ouputs of INTEGRATOR prototype with these models, while ensuring comparable model inputs, as described in the protocol for model comparison, will allow a model structure uncertainty analysis.

9 Uncertainty analyses/quantification with the final INTEGRATOR model

The final INTEGRATOR model will include more aspects than the prototype, such as C/N interactions and most likely a more detailed description of the CO_2 and CH4 emissions from natural soils. It is intended to redo an UQ for that model version, while including uncertainties in categorical data (soil maps and land use maps). Furthermore, we then will take into account all Soil Typological Units (STU) of each Soil Mapping Unit (SMU) and may be also the uncertainty in the STU.

9 Time planning for the uncertainty analyses/quantification

INTEGRATOR prototype

Month 30 (July 2008): more detailed set-up of the UQ of the INTEGRATOR prototype on a European scale, including a description of the uncertainties in model inputs (means, standard deviations and distributions) and their correlations. Possibly also preliminary results.

Month 36 (Feb 2009): Results of the UQ of the INTEGRATOR prototype on a European scale, focusing on model inputs.

Month 42 (July 2009): Comparison of the UQ of the INTEGRATOR prototype with (preliminary) UQs of selected detailed ecosystem models. Draft paper on the results

INTEGRATOR final version (first ideas)

Month 54 (July 2010): Results of the UQ of the INTEGRATOR model on a European scale, focusing on model inputs.

Month 60 (Feb 2011): Comparison of the UQ of the INTEGRATOR prototype with UQs of selected detailed ecosystem models. Draft paper on the results.