AqYield-NC model documentation : Extension of the AqYield soil-crop model for simulating microbial processes involved in soil nitrogen and carbon fluxes in the MAELIA platform

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Summary:

This document describes the soil subpart of the AqYield-NC model. AqYield-NC is an extension of the soil-crop model AqYield developed in the **MAELIA platform** (http://maelia-platform.inra.fr) to simulate nitrogen (N) and carbon (C) dynamics in the soil-crop system. First, a brief description of the two previously published versions of the model (*i.e.* **AqYield and AqYield-N**) is provided in **section 1**. The modified and new formalisms describing the simulated soil processes in **AqYield-NC** are then detailed in **section 2**. The calculations of some **environmental indicators** based on variables simulated in MAELIA are also provided in **section 3**.

MAELIA

Contents

1 Previous model versions

1.1 AqYield soil-crop model (2015-2018)

The first model version is described in Constantin et al. (2015) and in Tribouillois et al. (2018). AqYield is a soil-crop model simulating yields of several crops and water balance in soil at a daily time-step. The model considers soil characteristics (clay content, depth, maximum available water content), daily weather (rainfall, temperature and potential evapotranspiration), crop characteristics and agricultural practices (*e.g.* sowing and harvest dates, tillage, irrigation), with a total of 15 input data needed.

Soil water dynamics are simulated by calculating daily evaporation, crop transpiration and drainage. Crop aerial development is simulated using a crop coefficient (Kc) and root exploration is simulated by the growth of the associated soil available water content. AqYield does not simulate biomass production. Yields are calculated at harvest as a function of a local potential yield and water stress index over the entire development cycle of the crop.

Details on model equations are provided in Appendix A in Constantin et al. (2015) and Tribouillois et al. (2018).

1.2 AqYield-N (2020)

A model version called AqYield-N based on simple formalisms and requiring low input data was developed in order to predict nitrogen leaching from crop fields. Details on this model version are provided in Tribouillois et al. (2020). This version includes a redefined representation of soil compartments for N fluxes and additional modules to simulate nitrate transfers, crop N uptake and N inputs into the soil. In AqYield-N, crop yields are calculated at harvest as a function of a local potential yield and the highest stress among both water and N stresses.

The integration of the N module in AqYield led to a redefined representation of soil compartments into superimposed soil layers (see **Figure 1A**) instead of nested compartments in the initial version for water simulations. In the version of AqYield-N integrated in the MAELIA platform, the soil is subdivided in 3 compartments i) the biologically active layer w which extends from 0 cm to a depth ranging generally from 20 to 40 cm (30 cm by default), ii) the dynamic layer r which extends from the bottom of the layer w to the rooting depth and iii) the layer p which extends from the rooting depth to the bottom of the soil.

The initial amount of soil mineral nitrogen (SMN) in each layer is provided as input data. Mineral N coming from fertilization and from mineralization of soil organic N and crop residues are pooled into SMN of layer w. N taken up by crops can be retrieved from layers w and r. SMN is transferred with water transfers between layers (w to r, r to p) and SMN is leached with drainage ($N_{leaching}$ in kg N per ha) from layer p when soil water in p exceeds field capacity. SMN is homogeneously available in each layer and is the result of the balance between these different processes, as detailed in Tribouillois et al. (2020). Newly integrated soil processes and variables in AqYield-NC are shown in **Figure 1B** and detailed in the following section 2.
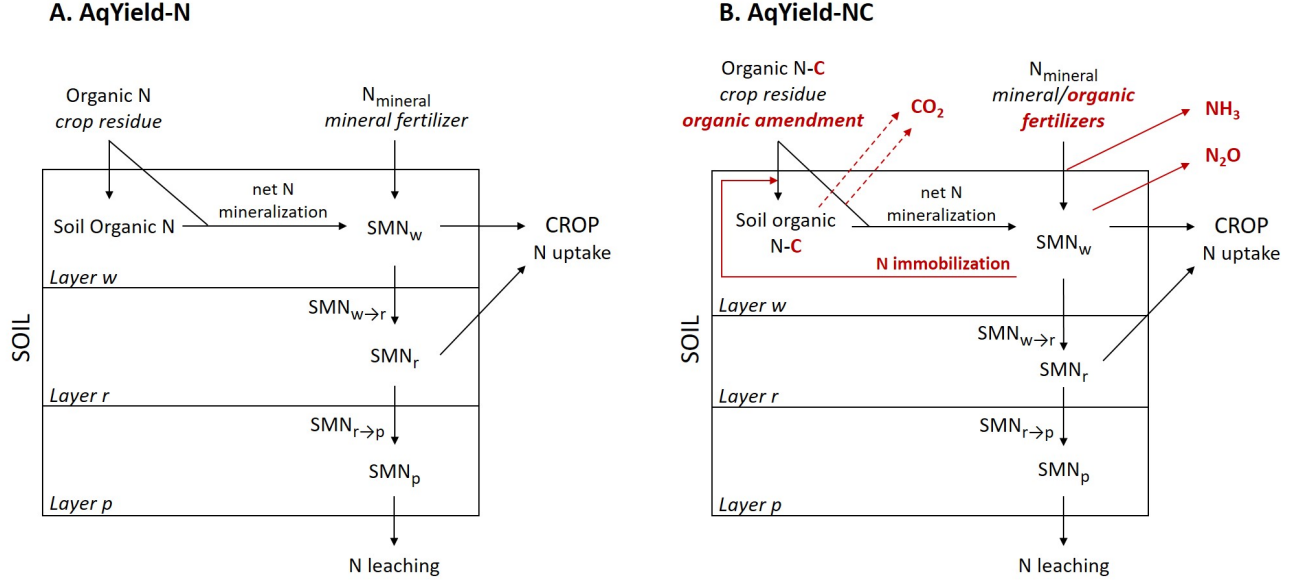
Figure 1: Description of the soil compartments and N fluxes in AqYield-N model (A) and processes and variables simulated in AqYield-NC (B). The red color indicates newly integrated processes and variables in AqYield-NC vs AqYield-N. Adapted from Tribouillois et al. (2020).

2 AqYield-NC: nitrogen and carbon fluxes

2.1 N and C inputs from crop residues and organic amendments

2.1.1 Crop residues

The method described in Clivot et al. (2019), which is based on the Bolinder approach (Bolinder et al., 2007), is applied to calculate aboveground (AG) and belowground (BG) C inputs from crop residues using crop yields or AG produced biomass for cover crops. The simulation of N acquired by the crop is then used to distribute N to the different plant parts (grain, straw, roots) according to their N contents and C/N ratios.

For the main crop, the yield simulated by the model is directly used in the calculation. For cover crops, AG biomass is considered as yield and calculated from N acquired by the plant, by inverting the function used to describe critical dilution curves of N in AG biomass in the STICS model (Brisson et al., 2009; Brisson et al., 2003), as follows:

In STICS, critical N content Nc (%) is calculated as:

$$Nc = adil \cdot biomass^{-bdil} \tag{1}$$

with $adil = 6.05$ and $bdil = 0.34$ for mustard cover crop, biomass is in ton dry matter (DM) per ha.

Inverting the function to calculate plant biomass from plant N in kg N per ha ($N_{plant} = Nc \cdot biomass \cdot 1000/100$) returns:

$$biomass(Nc) = exp(ln(N_{plant}/10/adil)/(1 - bdil)) \tag{2}$$

Plant nitrogen nutrition index INN (with a lower threshold for this function set at 0.5) is used to correct the calculated biomass:

$$biomass(INN) = exp(ln(N_{plant}/10/adil/max(0.5, INN))/(1 - bdil)) \tag{3}$$

4

- **Calculation of C inputs**

Plant aboveground C in straw and stubble (C_{AG} in kg C per ha) is calculated according to simulated yield at harvest (in t at standard moisture per ha) and crop harvest index (*HI*, grain to total aerial biomass ratio) for the main crop:

$$C_{AG} = Yield \cdot DM_{content} \cdot \frac{1 - HI}{HI} \cdot AerialC_{content} \cdot 1000 \tag{4}$$

where $DM_{content}$ is the dry matter content (in g per g) of the product and $AerialC_{content}$ is the C content of straw and stubble (in g C per g DM).

For cover crops, aerial C is calculated as:

$$C_{AG} = biomass(INN) \cdot AerialC_{content} \cdot 1000 \tag{5}$$

Aboveground C inputs into the soil (C_{AGsoil} in t C per ha) depend on the fraction of C_{AG} (*Pss*) that is returned to the soil:

$$C_{AGsoil} = C_{aerial} \cdot Pss \tag{6}$$

Pss is equal to 1.0 when all crop residues are left in the field or equal to *Pse* when AG residues such as straw are exported.

For belowground input estimates ($biomass_{BG}$ in t per ha), biomass in roots is calculated using shoot-to-root ratios (*SR*):

$$biomass_{BG} = \frac{Yield \cdot DM_{content}}{SR \cdot HI} \tag{7}$$

Belowground C inputs (C_{BG} in kg c per ha) in the biologically active layer w are calculated as:

$$C_{BG} = biomass_{BG} \cdot RootC_{content} \cdot 1.65 \cdot (1 - beta^{Zw}) \cdot 1000 \tag{8}$$

where $RootC_{content}$ is the root C content (g C per g DM), the factor 1.65 corresponds to the assumption that $extrarootC = 0.65 \cdot rootC$ (Bolinder et al., 2007). For keeping the model as simple as possible, extra-root C (rhizodeposits and fine root turnover over the crop cycle) is added to root C at crop harvest. The crop specific factor *beta* is used in the asymptotic equation of Gale and Grigal (1987) to determine the cumulative input fraction from the soil surface to the bottom of layer w (*Zw* cm depth).

An alternative method is proposed for estimating belowground C inputs using fixed values for some specific crops ($RootC_{fixed}$ in t C per ha) instead of allometric relationships, *i.e.* non-proportional to AG primary production (more details in Clivot et al. (2019)).

- **Calculation of N inputs**

First, potential nitrogen contents (in kg N per ha) in grain ($Ngrain_{pot}$) and in remaining crop biomass ($Nbiomass_{pot}$) are calculated as follows:

$$Ngrain_{pot} = Yield \cdot DM_{content} \cdot grainN_{content}/100 \cdot 1000 \tag{9}$$

$$Nbiomass_{pot} = \frac{C_{AG} + C_{BG}}{C/N_{biomass}} \tag{10}$$

where $grainN_{content}$ is the average percentage of N in grain for a specific crop and $C/N_{biomass}$ is the average C to N ratio of crop biomass, assuming that C/N ratios in AG and BG parts do not differ.

Nitrogen in grain ($Ngrain$) and in remaining biomass ($Nbiomass$) expressed in kg N per ha are then calculated as follows:

$$Ngrain = \frac{Ngrain_{pot}}{Ngrain_{pot} + Nbiomass_{pot}} \cdot N_{plant} \tag{11}$$

$$Nbiomass = \frac{Nbiomass_{pot}}{Ngrain_{pot} + Nbiomass_{pot}} \cdot N_{plant} \tag{12}$$

where N_{plant} is the N acquired by the crop (in kg N per ha) simulated by the model. For cover crops, $Nbiomass = N_{plant}$.

The allocation of N in aboveground (N_{AG}) and belowground parts (N_{BG}) in kg N per ha is calculated following these equations:

$$N_{AG} = \frac{C_{AG}}{C_{AG} + C_{BG}} \cdot Nbiomass \tag{13}$$

$$N_{BG} = \frac{C_{BG}}{C_{AG} + C_{BG}} \cdot Nbiomass \tag{14}$$

Aboveground N inputs into the soil (N_{AGsoil} in kg N per ha) depend on the fraction of N_{AG} (Pss) that is returned to the soil:

$$N_{AGsoil} = N_{AG} \cdot Pss \tag{15}$$

For belowground N inputs, N_{BG} below the biologically active layer is considered to be negligible and all N_{BG} inputs are allocated to the layer w. The C to N ratio of aerial and root residue (C/N_{res}) is therefore calculated as:

$$C/N_{res} = \frac{C_{AG} + C_{BG}}{Nbiomass} \tag{16}$$

The parameters for the calculations of C and N inputs for each crop species simulated in the Versailles Plain are given in **Table 1** for main crops and in **Table 2** for winter cover crops.

Table 1: Plant parameter values for calculating carbon and nitrogen inputs into the soil from main crop residues.

Parameters	Barley	Fababean	Maize.grain	Maize.forage	Pea	Rapeseed	Sorghum	Soybean	Sunflower	Wheat
DM_content	0.85	0.86	0.85	1	0.91	0.91	0.85	0.86	0.91	0.85
AerialC_content	0.44	0.44	0.44	0.44	0.44	0.44	0.44	0.44	0.44	0.44
RootC_content	0.4	0.4	0.4	0.4	0.4	0.4	0.4	0.4	0.4	0.4
HI	0.51	0.53	0.54	0.96	0.57	0.25	0.42	0.32	0.33	0.49
Pse	0.4	0.4	0.3	1	0.4	0.45	0.3	0.4	0.2	0.4
beta	0.94	0.961	0.952	0.952	0.963	0.92	0.952	0.938	0.928	0.96
SR	9.5	4	5.6	5.6	5.7	4.9	11.7	5.2	5.7	6.8
RootC_fixed	0.644	0.739	1.167	1.238	0.511	1.174	0.638	1.062	0.904	0.846
CN_biomass	75	32.5	60	60	32.5	67.5	60	32.5	45	82.5
grainN_content	1.7	3.5	2	1.3	3.5	3	1.7	5	2.2	2

Units are detailed in the text part 2.1.1; for forage maize, grainN_content corresponds to the N content of harvested aerial biomass

Table 2: Plant parameter values for calculating carbon and nitrogen inputs into the soil from cover crop residues.

Parameters	Mustard	Gramineous	Vetch
DM_content	1	1	1
AerialC_content	0.44	0.44	0.44
RootC_content	0.4	0.4	0.4
beta	0.928	0.96	0.928
SR	5.7	6.84	5.7
RootC_fixed	0.121	-	-
CN_biomass	22	25	15

Units are detailed in the text part 2.1.1

2.1.2 Organic amendments

- **Calculation of C inputs**

The model considers two fractions for the exogenous organic matter (EOM) amendments (Levavasseur et al., 2021): a labile fraction ($res1$) and a recalcitrant one ($res2$). The C inputs from the recalcitrant (C_{res2}) and the labile (C_{res1}) fractions (in kg C per ha) are calculated as:

$$C_{res2} = dose_{kg} \cdot EOMC_{content}/100 \cdot C2 \tag{17}$$

$$C_{res1} = dose_{kg} \cdot EOMC_{content}/100 \cdot (1 - C2) \tag{18}$$

where $dose_{kg}$ is the quantity of organic amendment applied (in kg fresh product per ha), $EOMC_{content}$ is the C content of EOM (in % of fresh matter) and $C2$ is the fraction of C in the recalcitrant part vs total C in EOM (in g C per g total C).

- **Calculation of N inputs**

The C to N ratio of the labile (C/N_{res1}) and recalcitrant (C/N_{res2}) fractions are calculated as:

$$C/N_{res1} = C/N_{res} \cdot aCN1 \tag{19}$$

$$C/N_{res2} = C2 \cdot C/N_{res} \cdot aCN1 \cdot C/N_{res}/(aCN1 \cdot C/N_{res} - (1 - C2) \cdot C/N_{res}) \tag{20}$$

where aCN1 is a parameter to compute the C to N ratio of the two fractions and C/N_{res} is the C to N ratio of the EOM organic fraction.

Organic Nitrogen in the labile (N_{res1}) and recalcitrant (N_{res2}) fractions (in kg N per ha) are calculated as:

$$N_{res1} = \frac{C_{res1}}{C/N_{res1}} \tag{21}$$

$$N_{res2} = \frac{C_{res2}}{C/N_{res2}} \tag{22}$$

Mineral Nitrogen input from EOM ($Nmin_{EOM}$ in kg N per ha) is calculated as:

$$Nmin_{EOM} = dose_{kg} \cdot EOMNmin/100 \tag{23}$$

where $EOMNmin$ is the percentage of mineral N in the organic amendment (in % of fresh matter)

The parameters for the calculations of C and N inputs for organic amendments are provided in **Table 3**.

Table 3: Parameter values for calculating carbon and nitrogen inputs into the soil for various exogenous organic matter (EOM) amendments.

EOM_type	EOMC_content	EOMNorg	CN_res	EOMNmin	Water_content	C2	aCN1
Urban sludges	1.53	0.17	8.9	0.02	94.8	0.47	1.21
Urban limed sludges	7.35	0.83	8.9	0.11	75	0.47	1.21
Dried paper mill sludge	7	0.26	26.9	0	72.5	0.47	1.21
Raw digestate	3.46	0.22	15.9	0.36	90	0.76	10
Digestate liquid fraction	1.5	0.13	12	0	95	0.76	10
Digestate solid fraction	10	0.37	26.7	0.01	50	0.76	10
Bovine manure	7.57	0.42	18.1	0.03	78.9	0.76	3.09
Sheep manure	12	0.64	18.8	0	69.7	0.76	3.09
Pig manure	14.08	0.57	24.9	0.08	67.1	0.75	1.14
Horse manure	16.85	0.5	33.6	0.02	58.6	0.52	10
Poultry manure	19.87	1.4	14.2	0.23	43.7	0.54	1.99
Chicken droppings	28.3	2.95	9.6	0.21	28.9	0.54	1.37
Bovine slurry	2.74	0.23	12	0.19	92.4	0.58	2.14
Pig slurry	2.05	0.17	11.9	0.15	95	0.6	5.25
Solid fraction of pig slurry	12.37	0.65	18.9	0.14	63.4	0.66	1.04
Fertylis	12.08	0.66	18.2	0.01	51.1	0.87	10
Green waste compost	13.98	0.77	18.2	0.02	43.4	0.87	10
Biowaste and green waste compost	13.21	1.01	13.1	0.02	37.7	0.84	10
Green waste and sludge compost	12.64	0.93	13.6	0.11	50.8	0.82	5.58
Municipal solid waste compost	16.62	0.83	20.1	0.05	34.3	0.56	1.65
Composted animal manure	11.59	0.78	14.9	0.05	64	0.67	2.07

Units are in % of fresh matter applied for EOMC_content, EOMNorg, EOMNmin and Water_content; and in g C per g of total C for C2

2.2 Microbial transformations of N and C

In AqYield-NC, the decomposition of soil organic matter (SOM) and fresh organic residues (crop residues, organic amendments) as well as nitrous oxide emissions are simulated daily in the biologically active layer w. Each soil tillage event mixes homogeneously SOM and organic residues between the soil surface and the tillage depth. As in AqYield-N, SMN is homogeneously available for microbial processes in the layer w for the sake of simplification. Ammonia volatilization is calculated using emission factors when fertilizers or organic amendments are applied on the soil surface.

2.2.1 Mineralization of soil organic matter

The mineralization of SOM is calculated as in the standard version 9.2 of the STICS model (Brisson et al., 2003). Initial soil organic carbon (SOC) and nitrogen (SON) stocks in layer w (expressed in kg organic C or N per ha) are calculated following Poeplau et al. (2017):

$$SOC = \frac{OM_{content}}{1.72} \cdot Zw \cdot BD \cdot (1 - Rf/100) \cdot 1000 \tag{24}$$

$$SON = \frac{SOC}{C/N_{soil}} \tag{25}$$

where, $OM_{content}$ is soil organic matter content (%), Zw is the soil depth of layer w (cm), BD is the bulk density of fine earth (g per cm^3), Rf is the volumetric fraction of rock fragments and C/N_{soil} is the C to N ratio of SOM.

SOM is divided into active (SOC_A and SON_A) and stable compartments (SOC_S and SON_S), the active part being decomposable and sustained by fresh organic inputs while the stable part is completely inert during the prediction time. SOM decomposition is simulated at the cm-scale in the layer w.

The size of the active pools is calculated as follows:

$$SOC_A = SOC \cdot (1 - Finert) \tag{26}$$
$$SON_A = SON \cdot (1 - Finert) \tag{27}$$

where $Finert$ is the initial fraction of the stable pool set by default at 0.65 (*i.e.* 65% of total SOM) for conditions of land-use with a long-term arable history. This value should depend on land use history and agricultural practices. More details on the setting of $Finert$ can be found in Clivot et al. (2019).

In each cm z over the layer w, $DSON_A$ *i.e.* the daily mineralization of SON_A (in kg N per ha per day) depends on environmental functions of soil characteristics (Clivot et al., 2017), temperature and soil moisture:

$$DSON_A(z) = -K \cdot SON_A(z) \cdot fmodP \tag{28}$$
$$\tag{29}$$

where fmodP is a factor modulating the priming effect on SOM mineralization (by default set at 1.0, see part 2.2.2), K is the actual mineralization rate calculated with environmental functions as follows:

$$K = Kpot \cdot f(T) \cdot f(H) \tag{30}$$
$$Kpot = 0.7 \cdot f(Clay) \cdot f(CaCO_3) \cdot f(pH) \cdot f(C/N) \tag{31}$$

$f(T)$ is a function of mean daily air temperature T (°C):

if $T \geq 0$,

$$f(T) = \frac{25}{1 + 145 \cdot exp(-0.12 \cdot T)} \tag{32}$$

if $T < 0$, $f(T) = 0$

$f(H)$ is a function of soil moisture calculated from the soil available water content (AWC in mm):

$$f(H) = \frac{(AWC + SWC_{pwp}) - (0.3 \cdot SWC_{fc})}{(1 - 0.3) \cdot SWC_{fc}} \tag{33}$$

where SWC_{pwp} and SWC_{fc} are soil water content at permanent wilting point and at field capacity (in mm), respectively.

Functions $f(Clay)$ and $f(CaCO_3)$ are describing the effects of *clay* and $CaCO_3$ contents (in %) on SOM mineralization, respectively:

$$f(Clay) = exp(-2.519 \cdot clay \cdot 10/1000) \tag{34}$$

$$f(CaCO_3) = \frac{1}{1 + 1.5 \cdot CaCO_3 \cdot 10/1000} \tag{35}$$

Functions $f(pH)$ and $f(C/N)$ are describing the effects of soil pH and C to N ratio C/N_{soil} on SOM mineralization:

$$f(pH) = exp(-0.112 \cdot (pH - 8.5)^2) \tag{36}$$

$$f(C/N) = exp(-0.06 \cdot (C/N_{soil} - 11)^2) \cdot 0.8 + 0.2 \tag{37}$$

In each cm z over the layer w, the daily mineralization $DSOC_A$, *i.e.* C outputs from SOC_A (in kg C per ha per day) is calculated as:

$$DSOC_A(z) = DSON_A(z) \cdot C/N_{soil} \tag{38}$$

Over the biologically active layer w (0-Zw cm depth):

- The daily C outputs $DSOC$ (in kg organic C per ha per day) from SOC are calculated as:

$$DSOC = \sum_{z=1}^{Zw} DSOC_A(z) \tag{39}$$

- Daily N mineralized from SOM $DNmin_{SOM}$ (in kg N per ha per day) is calculated as:

$$DNmin_{SOM} = \sum_{z=1}^{Zw} -DSON_A(z) \tag{40}$$

2.2.2 Mineralization of fresh organic residues

The decomposition of crop residues and organic amendments is simulated daily once incorporated into the soil by a tillage event. The humification of these products (*i.e.* processing into SOM) is simulated at the cm-scale and is considered to be homogeneous throughout their burial depths.

2.2.2.1 Mineralization of crop residues

The mineralization of crop residues is simulated as in the research version of the STICS model (release 2432) based on the equations from Nicolardot et al. (2001) and the parameterization from Justes et al. (2009) (see also (Brisson et al., 2009)), but with additional steps when mineral N becomes limiting for microbial processing of organic residues.

The C and N fluxes depend on the C to N ratio of the different compartments: residue (C/N_{res}), zymogenous biomass (C/N_{bio}) and SOM (C/N_{soil}); the decomposition rate constants of both residues ($Kres$) and
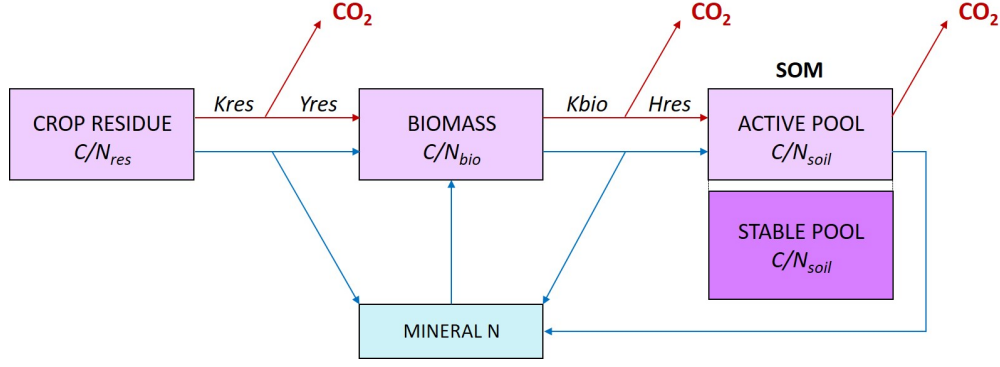
Figure 2: Description of the crop residue decomposition model. Red lines indicate carbon fluxes and blue ones nitrogen fluxes. SOM = Soil Organic Matter. Adapted from Nicolardot et al. (2001).

Table 4: Parameter values used for simulating the decomposition of crop residues.

Residue_type	AKres	BKres	AWb	BWb	CWb	AHres	BHres
Aerial	0.1	0.76	15.35	-76	7.8	0.73	10.2
Root	0.03	1.17	15.4	-80	7.8	0.78	25.9

zymogenous biomass ($Kbio$); two partition parameters ($Yres$ and $Hres$); air temperature and soil moisture; and mineral N availability which can affect the decomposition at different steps when N becomes limiting (**Figure 2**).

Some parameters are constant ($Yres = 0.62$ and $Kbio = 0.0076$) or depend on C/N_{res}, *i.e.* the C to N ratio of the residue, as follows:

$$Kres = AKres + \frac{BKres}{C/N_{res}} \tag{41}$$

$$C/N_{bio} = max(CWb; AWb + \frac{BWb}{C/N_{res}}) \tag{42}$$

$$Hres = 1 - AHres \cdot \frac{C/N_{res}}{BHres + C/N_{res}} \tag{43}$$

Parameter values for the decomposition of aerial and root residues are detailed in **Table 4**.

The effects of air temperature (T in °C) and soil moisture (calculated from the soil available water content AWC in mm) on the decomposition of both the residue and the zymogenous biomass are simulated using $f(T_{res})$ and $f(H)$ functions, respectively:

if $T < 0$, $f(T) = 0$; if $T \geq 0$:

$$f(T_{res}) = \frac{12}{1 + 52 \cdot exp(-0.103 \cdot T)} \tag{44}$$

$$f(H) = \frac{(AWC + SWC_{pwp}) - (0.3 \cdot SWC_{fc})}{(1 - 0.3) \cdot SWC_{fc}} \tag{45}$$

where SWC_{pwp} and SWC_{fc} are soil water content at permanent wilting point and at field capacity (in mm), respectively.

Daily variations in kg per ha of N (DN_{res}) and C (DC_{res}) of the decomposing residue are calculated as:

$$DN_{res} = -Kres \cdot N_{res} \cdot f(T_{res}) \cdot f(H) \cdot fmodK \tag{46}$$

$$DC_{res} = -Kres \cdot C_{res} \cdot f(T_{res}) \cdot f(H) \cdot fmodK \tag{47}$$

where fmodK (set by default at 1.0) is a factor modulating the residue decomposition rate when N is limiting (see below).

Daily variations in kg per ha of N (DN_{bio}) and C (DC_{bio}) of the zymogenous biomass are calculated as:

$$DN_{bio} = -(\frac{Yres \cdot fmodY \cdot DC_{res}}{min(C/N_{bio} \cdot fNCbio; 25.0)}) - Kbio \cdot N_{bio} \cdot f(T_{res}) \cdot f(H) \cdot fmodB \tag{48}$$

$$DC_{bio} = -(Yres \cdot fmodY \cdot DC_{res}) - Kbio \cdot C_{bio} \cdot f(T_{res}) \cdot f(H) \cdot fmodB \tag{49}$$

where $fmodY$, $fNCbio$ and $fmodB$ (set by default at 1.0) are modulating factors when N is limiting (see below).

The rate of humified organic matter formation, *i.e.* the C (DC_{hum}) and N (DN_{hum}) flows from decomposing zymogenous biomass to active SOM (in kg C or N per ha and per day) are calculated as:

$$DC_{hum} = Kbio \cdot Hres \cdot Cbio \cdot f(T_{res}) \cdot f(H) \tag{50}$$

$$DN_{hum} = \frac{Kbio \cdot Hres \cdot Cbio \cdot f(T_{res}) \cdot f(H) \cdot fmodH}{C/N_{soil}} \tag{51}$$

where $fmodH$ (set by default at 1.0) is a modulating factor of the C to N ratio of humified biomass when N is limiting (see below).

Humified C from zymogenous biomass ($HumC$ in kg organic C per ha per day) coming from the decomposition of n residue r in the layer w is calculated as:

$$HumC = \sum_{r=1}^{n} DC_{hum}(r) \tag{52}$$

- **Mineral N balance and N limitation for residue decomposers**

Net N mineralization resulting from the decomposition ($DNmin_{res}$) of n residue r in the layer w is calculated as:

$$DNmin_{res} = \sum_{r=1}^{n} -DN_{res}(r) - DN_{bio}(r) - DN_{hum}(r) \tag{53}$$

If $DNmin_{res} < 0$, a microbial demand for mineral N ($Ndemand_{mic}$) in the layer w is defined as:

$$Ndemand_{mic} = |DNmin_{res}| \tag{54}$$

Mineral N available for decomposers and plants in the layer w ($AvailSMN_w$ in kg N per ha) is calculated each day as the sum of initial SMN ($SMN_w ini$, *i.e* SMN_w at the end of the previous day) and N mineralized from SOM:

$$AvailSMN_w = SMN_w ini + DNmin_{SOM} \tag{55}$$

Each day, the potential Nitrogen demands in layer w from both the crop ($Ndemand_{cropW}$) and the decomposers ($Ndemand_{mic}$) are confronted to $AvailSMN_w$:

If $Ndemand_{crop} + Ndemand_{mic} \leq AvailSMN_w$ then the demands are satisfied.

If $Ndemand_{cropW} + Ndemand_{mic} > AvailSMN_w$ then the potential demands are used to calculate a reduced uptake of N in order to define actual N available for both decomposers ($Navail_{mic}$) and the crop ($Navail_{crop}$) as follows:

$$Navail_{mic} = \frac{Ndemand_{mic}}{Ndemand_{cropW} + Ndemand_{mic}} \cdot AvailSMN_w \tag{56}$$

$$Navail_{crop} = \frac{Ndemand_{crop}}{Ndemand_{cropW} + Ndemand_{mic}} \cdot AvailSMN_w \tag{57}$$

In case of mineral **N limitation for microbial decomposers**, *i.e.* $Ndemand_{mic} > Navail_{mic}$, different **cascading steps (up to 6 levels)** using modulating factors impacting microbial activities can be activated until the limitation is removed. These different steps are described below. The decomposition of residue and SOM is simulated at the end of each step with updated parameters and $Ndemand_{mic}$ is confronted again to $Navail_{mic}$.

If $Ndemand_{mic} \leq Navail_{mic}$, the updated parameterization is kept for the running day, but if $Ndemand_{mic} > Navail_{mic}$ then the following step is processed and so on, with cumulated effects for all the steps that are reached.

1. The decomposition rates of residue ($Kres$) and zymogenous biomass ($Kbio$) are reduced by the means of the predefined modulating factors with updated parameter values for $fmodK = 0.25$ and $fmodB = 0.5$ *vs* a value of 1.0 for both factors when N is not limiting.

2. The C to N ratio of the newly formed zymogenous biomass (C/N_{bio}) is increased using the factor $fNCbio$. Nitrogen potentially assimilated by the biomass ($DN_{bio}in$) is first calculated and cumulated for all residues ($SumDN_{bio}in$) as:

$$DN_{bio}in = -\left(\frac{Yres \cdot fmodY \cdot DC_{res}}{min(C/N_{bio} \cdot fNCbio; 25.0)}\right) \quad (58)$$

$$SumDN_{bio}in = \sum_{r=1}^{n} DN_{bio}in(r) \quad (59)$$

Then, if $SumDN_{bio}in > 10^{-6}$, the modulating factor $fNCbio$ is calculated as:

$$fNCbio = \frac{SumDN_{bio}in}{SumDN_{bio}in + Navail_{mic} + DNmin_{res}} \quad (60)$$

3. The C to N ratio of biomass humified into SOM is increased with a decrease in the factor $fmodH = 0.5$.

4. A priming effect on SOM mineralization is activated with changes in $fmodP$ calculated as follows:

$$fmodP = min\left(\frac{DNmin_{SOM} - DNmin_{res} - Navail_{mic}}{DNmin_{SOM}}; 3.0\right) \quad (61)$$

5. The assimilation yield of residue into microbial biomass ($Yres$) is reduced using $fmodY = 0.5$.

6. Finally, the residue decomposition is stopped by setting $fmodK$ at a value of 0.0.

The mineral N balance in the layer w resulting from the decomposition of both residues and SOM and from the crop N uptake ($SMN_w postMin$) is calculated as:

$$SMN_w postMin = SMN_w ini + DNmin_{res} + DNmin_{SOM} - Nuptake_{cropW} \quad (62)$$

where $Nuptake_{cropW}$ is the N assimilated by the crop in the layer w, with $Nuptake_{cropW} = Navail_{crop}$ in situation of N limitation. $SMN_w postMin$ is further used to calculate nitrous oxide emissions by denitrification (part 2.2.3.2).

At the **late stage of the residue decomposition**, when $N_{res} < 0.1$ and associated $N_{bio} < 1.0$, remaining C and N pools ($N_{res}; N_{bio}; C_{res}; C_{bio}$) are directly incorporated into active SOM and the **residue is removed**.

2.2.2.2 Mineralization of organic amendments

The decomposition of the labile fraction of EOM amendments is relatively similar to that of crop residues with constant parameters ($C/N_{bio1} = 7.0$, $Kbio = 0.0076$ and $Hres1 = 0.88$) and with specific parameters for the decomposition rate constant of the labile fraction of organic residues ($Kres1$) and its assimilation yield
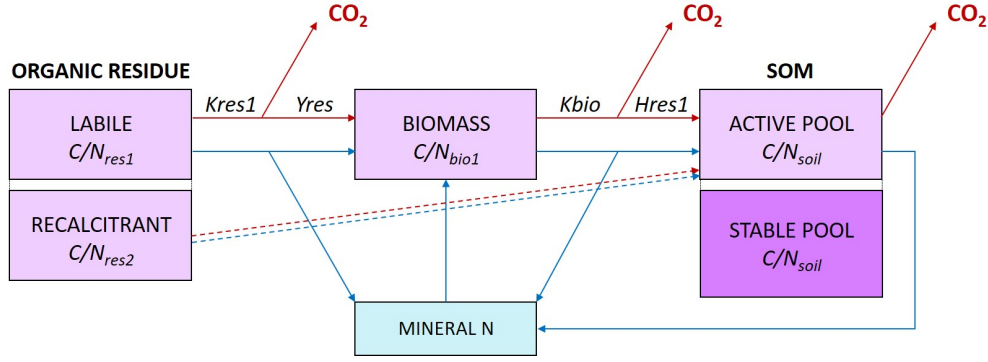
Figure 3: Description of the organic residue decomposition model. Red lines indicate carbon fluxes and blue ones nitrogen fluxes. Dotted lines show the direct incorporation of the recalcitrant fraction of organic amendment into SOM. SOM = Soil Organic Matter. Adapted from Nicolardot et al. (2001) and Levavasseur et al. (2021).

into the zymogenous microbial biomass ($Hres1$) as described in the M2 method proposed in Levavasseur et al. (2021). The calculation of the C to N ratio of organic residue fractions (C/N_{res1} and C/N_{res2}) is described in part 2.1.2. The decomposition rate constant of the recalcitrant fraction being relatively close to that of active SOM (Levavasseur et al., 2021), the recalcitrant pool of the organic amendment is directly moved into active SOM once incorporated into the soil (**Figure 3**).

Parameter values for the decomposition of different types of organic amendments are detailed in **Table 5**.

2.2.3 Nitrogen gaseous emissions

2.2.3.1 Ammonia volatilization

The approach developed in the INDIGO-N v.3 method (Avadi et al., 2020) is adapted in AqYield-NC for calculating ammonia volatilization (N_{NH_3} in kg N-NH$_3$ per ha) for each fertilizer type, based on emission factors (EF) from the EMEP/EEA air pollutant emission inventory guidebook 2019 and from Brockmann et al. (2018) and using correction factors (Cor_{NH_3}) for organic amendments.

- For mineral fertilizers, N_{NH_3} is calculated as:

$$N_{NH_3} = doseN_{kg} \cdot EF \cdot 14/17 \tag{63}$$

where $doseN_{kg}$ is the dose of N applied in kg per ha, EF depending on the fertilizer type and soil pH (**Table 6**). Emission Factors from the EMEP/EEA 2019 are used for most fertilizer types, excepting for urea for which the EF values from the 2013 report were kept, these latter being closer than ammonia emission values expected in France (Ramanantenasoa et al., 2018).

- For organic fertilizers, N_{NH_3} is calculated as:

$$N_{NH_3} = Nmin_{EOM} \cdot EF \cdot Cor_{NH_3} \tag{64}$$

where $Nmin_{EOM}$ is the mineral N in the organic amendment (see part 2.1.2) in kg N per ha, EF depending on the fertilizer type (**Table 7**). The correction factor Cor_{NH_3} depends on the fertilizer form: i) for solid organic fertilizer, Cor_{NH_3} depends on the timing of incorporation into the soil with values of 0.2, 0.5 and 1.0 for the day of amendment, one day after amendment and later, respectively ; ii) for liquid organic amendments, Cor_{NH_3} depends on the spreading technology used with values of 0.25, 0.5 and 1.0 for deep/shallow injections, trailing shoe and broadcaster, respectively.

Table 5: Parameter values used for simulating the decomposition of organic residues.

EOM_type	Kres1	Yres
Urban sludges	0.072	0.4
Urban limed sludges	0.072	0.4
Dried paper mill sludge	0.072	0.4
Raw digestate	0.024	0.25
Digestate liquid fraction	0.024	0.25
Digestate solid fraction	0.024	0.25
Bovine manure	0.025	0.32
Sheep manure	0.025	0.32
Pig manure	0.011	0.35
Horse manure	0.028	0.31
Poultry manure	0.055	0.34
Chicken droppings	0.077	0.1
Bovine slurry	0.062	0.39
Pig slurry	0.048	0.1
Solid fraction of pig slurry	0.036	0.57
Fertylis	0.005	0.6
Green waste compost	0.005	0.6
Biowaste and green waste compost	0.005	0.5
Green waste and sludge compost	0.005	0.6
Municipal solid waste compost	0.059	0.5
Composted animal manure	0.005	0.44

Table 6: Emission factors (EF) for ammonia emissions from mineral fertilizers

Fertilizer_type	EF_normal_pH	EF_high_pH
AH	0.020	0.036
AN	0.016	0.033
AP	0.051	0.094
AS	0.092	0.170
CAN	0.008	0.017
NK	0.022	0.033
NPK	0.067	0.094
NP	0.067	0.094
N solutions	0.100	0.097
Urea	0.243	0.243

Emission factors are expressed in kg NH3 per kg N applied; high pH is pH > 7.0

Table 7: Emission factors (EF) for ammonia emissions from organic fertilizers

EOM_type	EF	Form
Urban sludges	0.5	liquid
Urban limed sludges	0.5	solid
Dried paper mill sludge	0.5	solid
Raw digestate	0.7	solid
Digestate liquid fraction	0.6	liquid
Digestate solid fraction	0.8	solid
Bovine manure	0.8	solid
Sheep manure	0.7	solid
Pig manure	0.6	solid
Horse manure	0.7	solid
Poultry manure	0.4	solid
Chicken droppings	0.4	solid
Bovine slurry	0.5	liquid
Pig slurry	0.35	liquid
Solid fraction of pig slurry	0.8	solid
Fertylis	0.8	solid
Green waste compost	0.8	solid
Biowaste and green waste compost	0.8	solid
Green waste and sludge compost	0.8	solid
Municipal solid waste compost	0.8	solid
Composted animal manure	0.8	solid

Emission factors are expressed in kg N-NH3 per kg of mineral N applied

2.2.3.2 Nitrous oxide emissions

Nitrous oxide emissions (N_{N_2O} in kg N-N$_2$O per ha) by nitrification and denitrification processes are calculated using equations from the N$_2$O module of the decision support tool Syst'N (Parnaudeau et al., 2012) with additional parameters from the STICS model for denitrification (Léonard, 2016).

Nitrous oxide emissions by **nitrification** $N_{N_2O}Nit$ are calculated as a fraction (0.06%) of net N mineralized from the decomposition of crop residues, organic amendment and SOM (Garrido et al., 2002):

$$N_{N_2O}Nit = 0.0006 \cdot (DNmin_{res} + DNmin_{SOM}) \tag{65}$$

The calculation of nitrous oxide emissions by **denitrification** $N_{N_2O}Denit$ is adapted from equations of the NOE model (Hénault et al., 2005) and depends on temperature, soil moisture, pH and mineral N content in the layer w ($SMN_w preDenit$), the latter resulting from the following balance:

$$SMN_w preDenit = SMN_w postMin - N_{N_2O}Nit \tag{66}$$

Nitrous oxide emissions by denitrification ($N_{N_2O}Denit$) depend on the actual denitrification (Da in kg N per ha):

$$N_{N_2O}Denit = ratiodenit \cdot Da \tag{67}$$

where $ratiodenit$ is the fraction of denitrified N emitted as N$_2$O.

- The actual denitrification (Da) is calculated using a denitrification potential (set at $Dp = 2.0$ kg N per ha and per day) and response functions to soil mineral N content ($f(SMN)$), water-filled pore space ($f(wfps)$), temperature ($f(T_{denit})$) and soil pH ($f(pH_{denit})$) as follows:

$$Da = Dp \cdot f(SMN) \cdot f(wfps) \cdot f(T_{denit}) \cdot f(pH_{denit}) \tag{68}$$

Response function to SMN is calculated as:

$$f(SMN) = \frac{SMN_w preDenit \cdot 10^6 / SoilMass_w}{(SMN_w preDenit \cdot 10^6 / SoilMass_w) + 22} \tag{69}$$

where $SoilMass_w$ is the soil mass in kg soil per ha in the layer w calculated as follows:

$$SoilMass_w = Zw/100 \cdot BD \cdot 10000 \cdot (100 - Rf)/100 \cdot 1000 \tag{70}$$

Response function to water-filled pore space $f(wfps) = 0$ if $WFPS < 0.62$, else:

$$f(wfps) = (\frac{WFPS - 0.62}{1 - 0.62})^{1.74} \tag{71}$$

with WFPS calculated as :

$$WFPS = (\frac{((AWC + SWC_{pwp} + DrainedW)/Zw/10)}{porosity} \tag{72}$$

$$porosity = 1 - \frac{(2.65 \cdot Rf + BD \cdot (100 - Rf))/100}{2.65} \tag{73}$$

For the WFPS calculation, the daily drained water ($DrainedW$ in mm) is added to the soil water content ($AWC + SWC_{pwp}$) to account for the temporary near-saturation soil water content that can occur in the topsoil layer and which can not be simulated by the model, drainage occurring when the soil water content exceeds field capacity. The calculated WFPS is constrained to not exceed a value of 1.

For the response function to air temperature T, if $T < 11.0$°C:

$$f(T_{denit}) = exp(((T - 11) \cdot ln(89) - 9 \cdot ln(2.1))/10) \tag{74}$$

or if $T \geq 11.0$°C:

$$f(T_{denit}) = exp((T - 20) \cdot ln(2.1)/10) \tag{75}$$

For the response function to soil pH, $f(pH_{denit}) = 0$ if $pH < 4.0$, else $f(pH_{denit}) = 1$.

- The fraction of denitrified N emitted as N$_2$O *ratiodenit* (limited between 0 to 1) is calculated using response functions to water-filled pore space ($f(wfps)_r$), soil mineral N content ($f(SMN)_r$) and soil pH ($f(pH_{denit})_r$) as detailed in Léonard (2016):

$$ratiodenit = \frac{f(pH_{denit})_r}{f(wfps = 0.815)_r} \cdot f(wfps)_r \cdot f(SMN)_r \tag{76}$$

$$f(pH_{denit})_r = -(\frac{1}{9.2 - 5.6}) \cdot pH_{soil} + 2.556 \tag{77}$$

$$f(wfps)_r = 1 - \frac{WFPS - 0.62}{1 - 0.62} \tag{78}$$

$$f(SMN)_r = \frac{SMN_w preDenit \cdot 10^6/SoilMass_w}{(SMN_w preDenit \cdot 10^6/SoilMass_w) + 1} \tag{79}$$

with $f(wfps)_r = 1$ when $WFPS < 0.62$.

Total nitrous oxide emissions (N_{N_2O} in kg N-N$_2$O per ha) are calculated as:

$$N_{N_2O} = N_{N_2O}Nit + N_{N_2O}Denit \tag{80}$$

Denitrification also leads to **N$_2$ losses** ($N_{N_2}Denit$ in kg N-N$_2$ per ha) which can be calculated as:

$$N_{N_2}Denit = Da - N_{N_2O}Denit \tag{81}$$

3 AqYield-NC: environmental indicators

Processes and variables newly simulated in the AqYield-NC extension allow calculating some agro-environmental indicators related to C and N cycles to assess cropping system impacts at the plot scale. The calculation of the indicators described in this section are integrated in the MAELIA platform which provides them as model outputs.

3.1 Nitrogen losses

Nitrogen losses ($Nlosses$ in kg N per ha) can be calculated by combining N losses through mineral N leaching ($N_{leaching}$ already simulated in AqYield-N), ammonia volatilization (N_{NH_3}), nitrous oxide emissions (N_{N_2O}) and N_2 losses by denitrification ($N_{N_2}Denit$):

$$Nlosses = N_{leaching} + N_{NH_3} + N_{N_2O} + N_{N_2}Denit \tag{82}$$

3.2 Soil organic carbon dynamics

Soil organic carbon dynamics SOC_{dyn} in the biologically active layer w (in kg organic C per ha and per day) is the balance between the humified organic matter formation ($HumC$) from decomposing zymogenous biomass and the SOC outflow $DSOC$, *i.e.* the C mineralized from SOM:

$$SOC_{dyn} = HumC + DSOC \tag{83}$$

3.3 Greenhouse gas balance

The greenhouse gas balance at the plot scale ($GHG_{balance}$ in kg eqCO$_2$ per ha per day) is calculated as follows:

$$GHG_{balance} = 296 \cdot \frac{44}{28} \cdot (N_{N_2O} + 0.01 \cdot N_{NH_3} + 0.0075 \cdot N_{leaching}) - \frac{44}{12} \cdot SOC_{dyn} + Ferti_{synthesis} \tag{84}$$

where $Ferti_{synthesis}$ (in kg CO$_2$ per ha) is the amount of CO$_2$ emitted for the synthesis of fertilizers calculated using the data from the GESTIM+ reference (2020).

For an EOM product, $Ferti_{synthesis}$ is calculated as:

$$Ferti_{synthesis} = \frac{dose_{kg}}{1000} \cdot CO2_{EOM} \tag{85}$$

For a mineral fertilizer, $Ferti_{synthesis}$ is calculated as:

$$Ferti_{synthesis} = doseN_{kg} \cdot CO2_N + doseP_{kg} \cdot CO2_P + doseK_{kg} \cdot CO2_K \tag{86}$$

where the doses are expressed in kg of organic amendment or element (N, P and K) and $CO2_{EOM}$, $CO2_N$, $CO2_P$ and $CO2_K$ are the climate change impact in kg eqCO$_2$ per ton EOM or kg nutrient applied (**Tables 8 and 9**).

3.4 Soil structure quality (SOC:Clay)

The SOC to clay ratio ($SOC : Clay$) is calculated as a proxy of soil structure quality as proposed by Johannes et al. (2017), a ratio of 1:8 (0.125) being the average for a very good quality structure, 1:10 (0.100) being suggested as a reasonable goal for farmers and 1:13 (0.077) being a ratio below which the structure quality needs improvement.

Table 8: Climate change impact (in kg eqCO2) for each ton of organic fertilizer produced

EOM_type	CO2_EOM
Urban sludges	24.6
Urban limed sludges	24.6
Dried paper mill sludge	411.1
Raw digestate	52
Digestate liquid fraction	52
Digestate solid fraction	52
Bovine manure	11.1
Sheep manure	11.1
Pig manure	11.1
Horse manure	11.1
Poultry manure	11.1
Chicken droppings	11.1
Bovine slurry	27
Pig slurry	27
Solid fraction of pig slurry	27
Fertylis	652.5
Green waste compost	652.5
Biowaste and green waste compost	652.5
Green waste and sludge compost	652.5
Municipal solid waste compost	652.5
Composted animal manure	652.5

Table 9: Climate change impact (in kg eqCO2) for each kg of element produced for different types of mineral fertilizers

Fertilizer_type	CO2_N	CO2_P	CO2_K
AH	4.51	-	-
AN	3.97	-	-
AP	0	3.02	-
AS	4.51	-	-
CAN	4.18	-	-
NK	2.74	-	0.71
NPK	3.97	1.83	0.71
NP	3.97	1.83	-
N solutions	4.99	-	-
Urea	4.54	-	-
P	-	1.45	-
PK	-	1.45	0.71
K	-	-	0.71

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