MODELS INTEGRATED IN ECOINVENT LCI CALCULATION TOOL FOR CROP PRODUCTION

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1. Introduction

This document describes the models used to calculate the emissions from field activities as implemented in the ecoinvent LCI calculation tool for crop production. These models are aligned with those used in the World Food Life Cycle Database (WFLDB) as well as the World Apparel and Footwear Life Cycle Database (WALDB) and are also valid for the agricultural activities in the ecoinvent database. The texts below are taken partly from the guidelines of the WFLDB (Nemecek et al. 2015) but are repeated here for more convenience.

Model	source	Chapter
Ammonia (NH3) from mineral fertilizers application and manure spreading	(EEA (European Environment Agency) 2016)	2.1
Nitrous oxide (N2O)	IPCC (2006) Tier 1 for crop production	2.2
Nitrogen oxides (NOx, NO, NO2)	(EEA (European Environment Agency) 2016)	2.3
Nitrate leaching (NO3) (SQCB-NO3 model)	Faist Emmenegger et al 2009	2.4
Phosphorus (PO4) to water (SALCA-P model)	(Prasuhn 2006)	2.5
Erosion	Faist Emmenegger et al 2009 / (Ulrike Bos, Rafael Horn, Tabea Beck, Jan Paul Lindner 2016)	2.5.3
Calculation of BOD5, COD, DOC et TOC (emissions to groundwater)		2.6
Heavy metals to agricultural soil, surface water and groundwater (SALCA-heavy metal model)	(Freiermuth 2006)	2.7
Carbon dioxide from urea or lime application	(Eggleston et al. 2006)	2.8
Carbon dioxide, from land transformation	adaptation from Blonk consultants LUC tool, with link to ecoinvent v3 "land tenure" processes (compliant	2.9

		with LEAP and PAS 2050)	
Pesticides		2.10
Water emissions from irrigation	(Lévová et al. 2012)	2.11
Carbon dioxide uptake		2.11

These models result in following emissions:

1. Emissions to air (non-urban air or from high stacks):
   Ammonia (NH_3)
   Dinitrogen monoxide or nitrous oxide (N_2O)
   Nitrogen oxides (NO_x)
   Methane, biogenic (CH_4)
   Carbon dioxide, biogenic
   Carbon dioxide, fossil
   Carbon dioxide, from land transformation

2. Emissions to surface water:
   Phosphorus, surface water (P from erosion)
   Phosphate, surface water (PO_4^{3-} from run-off)
   Heavy metals: Cadmium (Cd), Chromium (Cr), Copper (Cu), Lead (Pb), Mercury (Hg), Nickel (Ni) and Zinc (Zn)

3. Emissions to groundwater:
   Nitrate (NO_3^-)
   Phosphate (PO_4^{3-})
   Heavy metals: Cadmium (Cd), Chromium (Cr), Copper (Cu), Lead (Pb), Mercury (Hg), Nickel (Ni) and Zinc (Zn)

4. Emissions to agricultural soil:
   Heavy metals: Cadmium (Cd), Chromium (Cr), Copper (Cu), Lead (Pb), Mercury (Hg), Nickel (Ni) and Zinc (Zn)
   Pesticides (if any applied)[1]

2. Description of the models

2.1. Ammonia (NH3)

Several methods are available for the estimation of NH3 emissions. The most widespread basis are the EMEP/EAA guidelines from the European Environment Agency, which are used to establish national emission inventories. The latest update of the methodology has been published in 2016 (EEA (European Environment Agency) 2016). The same methodology is also used in the AGRIBALYSE

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[1]

database (Colomb et al. 2014), with the difference that in AGRIBALYSE emission factors are taken from the EMEP/CORINAIR guidelines 2006 (EEA 2006), which represent a simplified approach. The ecoinvent V3.0 uses the Swiss Agrammon model for Swiss agricultural inventories, which is similar, but more detailed especially in the area of emissions from animal husbandry. The Agrammon model is a Tier-3 methodology for Switzerland and provides a number of correction factors, which can be used to represent specific situations. In the international context of the Ecoinvent LCI calculation tool for crop production, the EMEP/EAA guidelines are followed.

The emission factors for mineral fertiliser are taken from the EMEP guidelines 2016 ((EEA (European Environment Agency) 2016)).

Tab. 1: Emission factors for NH3 after the application of mineral N fertiliser ((EEA (European Environment Agency) 2016), 3.D Table 3-2) in function of the soil pH.

Fertilizer type (m)	cool climate (cf. IPCC 2006)		temperate climate (cf. IPCC 2006)		warm climate (cf. IPCC 2006)	
	EFa kgN/kg N soil pH<=7	EFb kgN/kg N soil pH>7	EFa kgN/kg N soil pH<=7	EFb kgN/kg N soil pH>7	EFa kgN/kg N soil pH<=7	EFb kgN/kg N soil pH>7
Ammonium sulphate (AS)	0.07	0.14	0.08	0.14	0.09	0.17
Ammonium nitrate (AN)	0.01	0.03	0.01	0.03	0.02	0.03
Calcium ammonium nitrate (CAN)	0.01	0.01	0.01	0.01	0.01	0.02
Anhydrous ammonia	0.02	0.03	0.02	0.03	0.02	0.04
Urea	0.13	0.14	0.13	0.14	0.16	0.17
Urea ammonium nitrate (UAN)	0.08	0.08	0.08	0.08	0.10	0.10
Di ammonium phosphate (DAP)	0.04	0.07	0.04	0.08	0.05	0.10
Mono ammonium phosphate (MAP)	0.04	0.07	0.04	0.08	0.05	0.10
Other complex NK, NPK fertilizer	0.04	0.07	0.06	0.08	0.05	0.10
Urea ammonium sulphate (UAS)	0.13	0.14	0.13	0.14	0.16	0.17

Source: EMEP guidebook 20(EEA (European Environment Agency) 2016)16, part 3D: Crop production and agricultural soils, Table 3.2

The emission is calculated as follows:

$NH_3 \quad = 17/14 * \sum_{m-1}^{M}\left(EFa_m * p + EFb_m * (1 - p)\right) * N_{min}$

where

NH_3 = ammonia emission after mineral fertiliser application [kg NH_3]

m = fertiliser type (M = number of fertiliser types)

EFa_m = emission factor on soils with pH<=7 [kg NH_3-N/kg N] (see Tab. 1)

EFb_m = emission factor on soils with pH>7 [kg NH_3-N/kg N] (see Tab. 1)

p   = fraction of soils with pH <= 7 [%/100]

N_{min} = mineral fertiliser application [kg N]

The conversion factor from N to NH_3 is 17/14.

- Dinitrogen monoxide or nitrous oxide (N_2O)

2.2. Nitrous oxide (N2O)

Nitrous oxide (N_2O) is produced during nitrification and denitrification processes and is a very powerful greenhouse gas. For nitrous oxide we are following IPCC guidelines ((Eggleston et al. 2006)) Tier 1 for crop production.

N_2O = 44/28 * (0.01 (N_{tot} + N_{cr} + N_{som} + 14/17*NH_3 + 14/46*NO_x) + 0.0075 * 14/62*NO_3)

N_2O = emission of N_2O [kg N_2O ha^{-1}]

N_{tot} = total nitrogen in mineral and organic fertiliser [kg N ha^{-1}]

N_{cr} = nitrogen contained in the crop residues [kg N ha^{-1}]

N_{som} = nitrogen from mineralisation of soil organic matter [kg N ha^{-1}]

NH_3 = losses of nitrogen in the form of ammonia [kg NH_3 ha^{-1}]

NO_x = losses of nitrogen in the form of nitrogen oxides [kg NO_2 ha^{-1}].

NO_3 = losses of nitrogen in the form of nitrate [kg NO_3 ha^{-1}].

N_2O released during decomposition of organic matter in the soil after land use change is a further source of emissions.

For flooded rice, the emission factor for direct emissions of N_2O is 0.003 (IPCC, 2006, Table 11.1, EF_{1FR}) instead of 0.01.

2.3. Nitrogen oxides (NO$_x$, NO, NO$_2$)

Nitrogen oxides stem mainly from the nitrification process. The importance of NO_x emissions from N fertiliser is relatively small compared to other sources. Therefore simple emission factors are used. The emission factor for the application of mineral and organic fertiliser (including animal manure) is:

- 0.018667 kg NO_x-N/kg N applied (EEA, 2016, 3.D Tab. 3-1, converted from NO to N: 0.04*14/30=0.018667)

The emission is calculated after subtraction of the N volatilized as NH_3.

EEA (2016) expresses the emissions of NO_x as NO, while in ecoinvent NO_x is calculated as NO_2. In order to be compatible with the latter, the emissions will be converted to NO_2. The conversion factor from N to NO_2 is 46/14.

2.4. Nitrate leaching to ground water

The SQCB-NO$_3$ model, a geographically unspecific and simple model, is used

, in: Faist Emmenegger *et al.* 2009).

Gaseous losses of NH$_3$, NO$_x$ and N$_2$O are subtracted from the amount of N applied in the fertilisers prior to the calculation of nitrate leaching.

The SQCB-NO$_3$ model is reported in Faist Emmenegger *et al.* (2009) and is an adaption of a formula developed by de Willigen (2000) and used and validated by Roy *et al*. (2003). The formula calculates the leaching of NO$_3$-N and is a simple regression model of the form:

$$N = 21.37 + \frac{P}{c*L}\left[0.0037*S + 0.0000601*N_{org} - 0.00362*U\right]$$

where:

N	= leached NO$_3$-N	[kg N/(ha*year)]
P	= precipitation + irrigation	[mm/year]
c	= clay content	[%]
L	= rooting depth	[m]
S	= nitrogen supply through fertiliser	[kg N/ha]
N$_{org}$	= nitrogen in organic matter	[kg N/ha]
U	= nitrogen uptake by crop	[kg N/ha]

The SQCB model provides relatively simple approaches to assess most of the required input parameters. P and C$_{org}$ are determined through the ecozone in which the crop is produced. The ecozones for the whole globe are defined and presented as maps in FAO (2001). Fix values for carbon content in the upper 30 cm of soil and for annual precipitation are assigned to each ecozone (see **Erreur ! Source du renvoi introuvable.**). More specific values can be used, where available. The carbon content in tonnes per 3000 m^3 (1 ha [area] * 30 cm [depth]) is converted into mass fraction by the formula:

C$_{org}$ [%] = C$_{org}$ [t/3000 m^3] * (1 / 1.3 t m^{-3}) * 100

In case of irrigation, the amount of irrigation water [mm] is added to the precipitation in order to obtain the parameter P. The amount of irrigation water is calculated according to section **Erreur ! Source du renvoi introuvable.**.

The annual precipitation and the irrigation are inputs from the user.

The carbon content is an average value per country (see Annex XX), the clay content c is defined by the average soil texture of a country (see Annex XX),.

The rooting depth for several crops is given in the SQCB report by Faist Emmenegger (2009). The missing values were taken from other literature. Values and sources are presented in the Annex XX

The nitrogen supply S is calculated from the total N application of mineral fertilisers and of soluble N in organic fertilisers after subtraction of the gaseous losses in form of NH$_3$, NO$_x$ and N$_2$O. The original model sources (de Willigen, 2000; Roy *et al*. 2003) do not make a clear distinction between mineral

and organic fertilisers. Since only the mineral (soluble) form of N is prone to leaching and for reasons of consistency with the SALCA-NO_3 model, only the soluble part of N in organic fertilisers is counted.

The nitrogen uptake U can be taken from Faist Emmenegger *et al.* (2009) or other sources (e.g. Flisch *et al.*, 2009) and are summarized in the annex. Linear adjustments must be made for different yields. In the case of legumes, only 40% of the values given in the SQCB report are considered as N uptake in order to reflect the fact, that the remaining 60% are fixed from the air and are not directly relevant to the balance of nitrogen supplied through fertilisers and mineralised from the soil organic matter (Schmid *et al.* 2000).

To calculate the organic nitrogen N_{org} in soil [kg N/ha] from the soil organic carbon content C_{org} [%] the following quantities are needed:

- soil volume V [m^3/ha]

V is taken to be 5000 m^3, which means that the upper 50 cm of soil are considered (according to pers. comm. J. Leifeld, ART, 2011), assuming the same carbon content for 30-50 cm depth as calculated above for 0-30 cm depth.

- bulk density D_b [kg/m^3]

Bulk density is taken to be 1300 kg/m^3, which is the standard value from the SQCB report.

- C/N ratio $r_{C/N}$ [dimensionless]

The C/N ratio is taken to be 11. This is the mean value of the range (10-12) determined through literature research (Batjes 2008; Scheffer 2002; Eggleston *et al.* 2006) and consultation of experts (pers. comm. J. Leitfeld, Agroscope).

- ratio of N_{org} to N_{tot} (total soil nitrogen) r_{Norg} [dimensionless]

The C/N ratio expresses the ratio of C_{org} and N_{tot}. The ratio r_{Norg} is needed calculate N_{org} from N_{tot}, which is calculated in a first step applying the C/N ratio. r_{Norg} is assumed to be 0.85 (Scheffer 2002).

- N_{org} is calculated by the formula:

$$N_{org} = \left(\frac{Corg}{100} \times V \times D_b \right) \div r_{C/N} \times r_{Norg}$$

N_{org} is the mass of organic nitrogen contained in the upper 50 cm of soil. Naturally only a fraction of this mass is mineralised and, hence, available for uptake by plants and leaching to the ground water. This fraction is determined by the mineralisation rate, which is 1.6% here and implicitly included in the regression coefficient (0.0000601) of the term N_{org}.

2.5. Phosphorus emissions to water

Three different paths of phosphorus emissions to water are distinguished:

- leaching of soluble phosphate (PO_4) to ground water (inventoried as "phosphate, to ground water"),
- run-off of soluble phosphate to surface water (inventoried as "phosphate, to surface water"),
- water erosion of soil particles containing phosphorus (inventoried as "phosphorus, to surface water").

Erosion by wind is not considered in these guidelines. However, in cases where wind erosion is important, it should be taken into account.

The emission models SALCA-P (Prasuhn 2006) developed by Agroscope are applied. The following factors are considered for the calculation of P emissions:

- type of land use
- type of fertiliser
- quantity of P in fertiliser
- type and duration of soil cover for the calculation of the soil erosion (C-factor).

For other factors, considered in the model SALCA-P, default values are used (Prasuhn 2006):

- distance to next river or lake
- topography
- chemical and physical soil properties
- drainage.

The model takes soil erosion, surface run-off and drainage losses to surface water and leaching to ground water into account.

The key factors of the model are listed below.

2.5.1. Phosphate leaching to ground water

P leaching to the ground water was estimated as an average leaching, corrected by P-fertilization:

$P_{gw} =$ $P_{gwl} * F_{gw}$

$P_{gw} =$ quantity of P leached to ground water [kg/(ha*a)]

$P_{gwl} =$ average quantity of P leached to ground water for a land use category [kg/(ha*a)], which is:
0.07 kg P/(ha*a) for arable land and
0.06 kg P/(ha*a) for permanent pastures and meadows.

$F_{gw} =$ correction factor for fertilization by slurry [dimensionless]

$F_{gw} =$ $1 + 0.2/80*P_2O_{5sl}$

$P_2O_{5sl} =$ quantity of P_2O_5 contained in the slurry or liquid sewage sludge [kg/ha]. The values of P_2O_5-content were taken from Flisch *et al.* (2009) or other national sources.

2.5.2. Phosphate run-off to surface water

Run-off to surface water was calculated in a similar way to leaching to ground water:

$P_{ro} =$ $P_{rol} * F_{ro}$

$P_{ro} =$ quantity of P lost through run-off to rivers [kg/(ha*a)]

$P_{rol} =$ average quantity of P lost through run-off for a land use category [kg/(ha*a)], which is
0.175 kg P/(ha*a) for arable land,
0.25 kg P/(ha*a) for intensive permanent pastures and meadows and
0.15 kg P/(ha*a) for extensive permanent pastures and meadows

$F_{ro} =$ correction factor for fertilization with P [dimensionless], calculated as:

$F_{ro} =$ $1 + 0.2/80 * P_2O_{5min} + 0.7/80 * P_2O_{5sl} + 0.4/80 * P_2O_{5man}$
$P_2O_{5min} =$ quantity of P_2O_5 contained in mineral fertiliser   [kg/ha]

P_2O_{5sl} = quantity of P_2O_5 contained in slurry or liquid sewage sludge   [kg/ha]

P_2O_{5man} = quantity of P_2O_5 contained in solid manure   [kg/ha]

The values of P_2O_5-content for slurry and manure were taken from Flisch *et al*. (2009) or other national sources.

2.5.3. Phosphorus emissions through water erosion to surface water

P emissions through erosion of particulate phosphorous to surface water were calculated as follows:

P_{er} = $S_{er} * P_{cs} * F_r * F_{erw}$

P_{er} =   quantity of P emitted through erosion to rivers [kg P/(ha*a)]

S_{er} =   quantity of soil eroded [kg/(ha*a)]

P_{cs} =   P content in the top soil [kg P/kg soil]. The average value of 0.00095 kg/kg was used.

F_r =   enrichment factor for P (-). The average value of 1.86 was used (Wilke & Schaub 1996). This factor takes account of the fact that the eroded soil particles contain more P than the average soil.

F_{erw} =   fraction of the eroded soil that reaches the river [dimensionless]. The average value of 0.2 was used.

The amount of eroded soil S_{er} is calculated using the universal soil loss equation as described in Faist Emmenegger *et al.* (2009), where the USLE (Universal Soil Loss Equation, Wischmeier and Smith 1978) is expressed as:

S_{er} = 1000 * R * k * LS * c1 * c2 * P

where

S_{er} = Potential long term annual soil loss [kg ha^{-1} yr^{-1}]

R = Erosivity factor [MJ mm ha^{-1} h^{-1} yr^{-1}]

k = Erodibility factor [t h MJ^{-1} mm^{-1}]

LS = Slope factor [-]

c1 = Crop factor [-]

c2 = Tillage factor [-]

P = Practice factor [-]

The erosivity factor R is computed according to the LANCA methodology (Bos et al. 2016 LANCA characterisation factors for Life Cycle Impact Assessment, Version 2.0), which compiles a set of formula depending on the climate zone.

Table 2 R-Factor approximation equations for the regarded climate zones

Climate zone	Equation	Source
Equatorial fully humid	$= -3172 + 7.562 * P$	(Mikhailava et al. 1995)
Equatorial monsoonal	$= -3172 + 7.562 * P$	(Mikhailava et al. 1995)
Equatorial summer dry	$= -669.3 + 7 * P - 2.719 * E$	(Mikhailava et al. 1995)
Equatorial winter dry	$= -3172 + 7.562 * P$	(Mikhailava et al. 1995)
Arid desert cold arid	$= 0.809 * P^{0.957} + 0.000189 * S^{6.285}$	(Naipal et al. 2015)
Arid desert hot arid	$= 0.0438 * P^{1.61}$	(Yu and Rosewell 1996)
Arid steppe cold arid	$= 10^{(0.0793 + 0.887 * \log(P) + 1.892 * \log(S) - 0.429 * \log(E))}$	(Naipal et al. 2015)
Arid steppe hot arid	$= 10^{(-7.72 + 1.595 * \log(P) + 2.068 * \log(S))}$	(Naipal et al. 2015)
Warm temperate fully humid hot summer	$= 10^{(0.524 + 0.462 * \log(P) + 1.97 * \log(S) - 0.106 * \log(E))}$	(Naipal et al. 2015)
Warm temperate fully humid warm summer	$= 10^{(-7.694 + 4.1407 + \log(P) - 2.586 * \log(S))}$	(Naipal et al. 2015)
Warm temperate fully humid cold summer	$= 10^{(-7.694 + 4.1407 + \log(P) - 2.586 * \log(S))}$	(Naipal et al. 2015)
Warm temperate summer dry hot summer	$= -944 + 3.08 * P$	(Cooper 2011)
Warm temperate summer dry warm summer	$= 98.35 + 3.55 * 10^{-4} * P^{1.987}$	(Naipal et al. 2015)
Warm temperate summer dry cold summer	$= -944 + 3.08 * P$	(Cooper 2011)
Warm temperate winter dry hot summer	$= -3172 + 7.562 * P$	(Mikhailava et al. 1995)

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Climate zone	Equation	Source
Warm temperate winter dry warm summer	$= -3172 + 7.562 * P$	(Mikhailava et al. 1995)
Warm temperate winter dry cold summer	$= -3172 + 7.562 * P$	(Mikhailava et al. 1995)
Snow fully humid hot summer	$= 10^{(-1.99 + 0.737 * \log(P) + 2.033 * \log(S))}$	(Naipal et al. 2015)
Snow fully humid warm summer	$= 10^{(-0.5 + 0.266 * \log(P) + 3.1 * \log(S) - 0.131 * \log(E))}$	(Naipal et al. 2015)
Snow fully humid cold summer	$= 10^{(-1.259 + 3.862 * \log(S))}$	(Naipal et al. 2015)
Snow fully humid extremely continental	$= 10^{(-1.259 + 3.862 * \log(S))}$	(Naipal et al. 2015)
Snow summer dry hot summer	$= 10^{(1.882 + 0.819 * \log(P))}$	(Naipal et al. 2015)
Snow summer dry warm summer	$= 10^{(2.166 + 0.494 * \log(P))}$	(Naipal et al. 2015)
Snow summer dry cold summer	$= 10^{(4.416 + 0.0594 * \log(P))}$	(Naipal et al. 2015)
Snow summer dry extremely continental	$= 10^{(4.416 + 0.0594 * \log(P))}$	(Naipal et al. 2015)
Snow winter dry hot summer	$= 38.5 + 0.35 * P$	(Lee and Lee 2006)
Snow winter dry warm summer	$= 38.5 + 0.35 * P$	(Lee and Lee 2006)
Snow winter dry cold summer	$= 10^{(1.882 + 0.819 * \log(P)}$	(Naipal et al. 2015)
Snow winter dry extremely continental	$= 10^{(1.882 + 0.819 * \log(P))}$	(Naipal et al. 2015)
Polar polar frost	$= 10^{(-10.66 + 2.43 * \log(P))}$	(Naipal et al. 2015)
Polar polar tundra	$= 10^{(-10.66 + 2.43 * \log(P))}$	(Naipal et al. 2015)

Where:

P = Average annual precipitation [mm/year]

E = Mean elevation [m]

S = Average annual precipitation / number wet days [mm/day]

The climate zone is entered by the user based on a map; the number of wet days per year is also given by the user.

The LS factor computation is based on the original equation described in Wischmeier and Smith (1978). The only adjustment consists in transforming the input data from the SI (International System of Units) units to the American metric system. Indeed this formula requires length in feet whereas the user types it in in meters.

$$LS_i = \begin{cases} \left(\dfrac{L_i * 3.28083}{72.6}\right)^{0.2} * (65.41 * (\sin(\dfrac{S_i}{100}))^2 + 4.56 * (\sin(\dfrac{S_i}{100})) + 0.065) & if & S_i < 1\% \\[2ex] \left(\dfrac{L_i * 3.28083}{72.6}\right)^{0.3} * (65.41 * (\sin(\dfrac{S_i}{100}))^2 + 4.56 * (\sin(\dfrac{S_i}{100})) + 0.065) & if & 1\% \le S_i < 3.5\% \\[2ex] \left(\dfrac{L_i * 3.28083}{72.6}\right)^{0.4} * (65.41 * (\sin(\dfrac{S_i}{100}))^2 + 4.56 * (\sin(\dfrac{S_i}{100})) + 0.065) & if & 3.5\% \le S_i \le 5\% \\[2ex] \left(\dfrac{L_i * 3.28083}{72.6}\right)^{0.5} * (65.41 * (\sin(\dfrac{S_i}{100}))^2 + 4.56 * (\sin(\dfrac{S_i}{100})) + 0.065) & if & S_i > 5\% \end{cases}$$

Where S_i is the slope of the segment i expressed in %, L_i is the length of the segment i expressed in meters and LS_i is the partial slope factor for the segment i. The factor 3.28083 is a conversion factor from meter to feet and 100 is a conversion factor related to the fact that the slope is expressed in %.

LS is then computed as the sum of all LS_i:

$$LS = \sum_{i=1}^{n} LS_i$$

Where n is the number of segments. Here, only one segment will be considered as default.

The K factor is calculated either from the Table 7-2 given by Faist Emmenegger *et al.* (2009) or taken from Table 5 in Panagos et al. (2014) for European countries and Table 4 for other countries, where the information about the soil class is not available (only the clay and sand content needed).

The c1 factor is taken from Table 7-3, c2 the factor from 7-4 and the P factor from Table 7-5 in Faist Emmenegger *et al.* (2009) or from other literature.

2.6. Calculation of BOD5, COD, DOC and TOC (emissions to groundwater)

The BOD5, COD, DOC and TOC emissions in groundwater are calculated as follow:

DOC = TOC = COD/2.7

BOD5 = 0.5*COD (for untreated waste water (default case), for other cases, see below)

The BOD5/COD ratio depends on the biodegradability of the organic material.

- At full biodegradability BOD = COD.
- For domestic wastewater values up to BOD5 = 0.75*COD can be found

- For food industries BOD5 = 0.9*COD.
- For wastewaters with low nutrient content relative to carbon, such as from chemical plants and in cleaned wastewaters, BOD5 = 0.2*COD and when having passed a nutrient elimination step BOD5 = 0.05*COD

2.7. Heavy metals emissions to agricultural soil, surface water and ground water

According to an analysis of the heavy metals[2] that are causing problems in agriculture (Kühnholz 2001), the following seven were selected:

- Cadmium (Cd)
- Chromium (Cr)
- Copper (Cu)
- Lead (Pb)
- Mercury (Hg)
- Nickel (Ni)
- Zinc (Zn)

No distinction is made between CrII and CrIII, only the sum of Cr flows is considered.

Typical heavy-metal content of agricultural and non-agricultural soils is given by Desaules & Dahinden (2000). Kühnholz (2001) gives a comparison of different emission factors and methods for calculating heavy metal balances.

The heavy metal emissions are calculated by SALCA-heavy metal (Freiermuth 2006). Inputs into farm land and outputs to surface water and groundwater are calculated on the basis of heavy metal input from seed, fertiliser, plant protection products and deposition from the air. Crop residues left on the field are not considered, since they do not leave the system. Average heavy metal contents for arable land, pastures, meadows and horticultural crops are used to calculate the amounts of heavy metals exported by soil erosion. The amount of eroded soil is the same as calculated for the P-emissions (see above). An allocation factor is used to distinguish between diffuse and agriculture-related introduction (Freiermuth 2006).

Three types of emissions are considered:

- Leaching of heavy metals to the ground water (always positive values)
- Emissions of heavy metals into surface waters through erosion of soil particles (always positive values)
- Emissions of heavy metals to agricultural soil (positive or negative values according to the results of the balance).

The following sources are used to calculate heavy-metal contents:

- Mineral fertiliser: Desaules & Studer (1993, p. 153), see Tab. 6,
- Farmyard manure: Menzi & Kessler (1998) and Desaules & Studer (1993, p. 152), see Tab. 7,

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[2] Heavy metals are metals with a specific weight greater than 5 g/cm^{3} (Source: http://chemistry.about.com/od/chemistryglossary/g/Heavy-Metal-Definition.htm).

- pesticides: FOAG (2014),
- biomass (seed and products from plant production): Houba & Uittenbogaard (1994, 1995, 1996 & 1997), von Steiger & Baccini (1990) and Wolfensberger & Dinkel (1997); Bennett et al. (2000) & for Nickel Teherani (1987) for rice; generic mean of biomass for cotton due to lack of data with mass allocation to fibre and seed (Freiermuth 2006); see Tab. 5.

Heavy metal emissions into ground and surface water (in case of drainage) are calculated with constant leaching rates as:

$M_{leach\ i} = m_{leach\ i} * A_i$

$M_{leach\ i}$ agricultural related heavy metal *i* emission

$m_{leach\ i}$ average amount of heavy metal emission (Tab. 2)

A_i allocation factor for the share of agricultural inputs in the total inputs for heavy metal *i*

Tab. 2: Heavy metal leaching to groundwater according to Wolfensberger & Dinkel (1997).

Leaching	Cd	Cu	Zn	Pb	Ni	Cr	Hg
mg/ha/year	50	3600	33000	600	n.a.	21200	1.3

Heavy metal emissions through erosion are calculated as follows:

$M_{erosion\ i} = c_{tot\ i} * S_{er} * a * f_{erosion} * A_i$

$M_{erosion}$ agricultural related heavy metal emissions through erosion [kg ha^{-1} a^{-1}]

$c_{tot\ i}$ total heavy metal content in the soil (Keller & Desaules 2001, see Tab. 3 [kg/kg])

S_{er} amount of soil erosion (see section 2.5.3) [kg ha^{-1} a^{-1}]

a accumulation factor 1.86 (according to Wilke & Schaub (1986) for P) [-]

$f_{erosion}$ erosion factor considering the distance to river or lakes with an average value of 0.2 (considers only the fraction of the soil that reaches the water body, the rest is deposited in the field) [dimensionless]

A_i allocation factor for the share of agricultural inputs in the total inputs for heavy metal *i* [dimensionless]

Tab. 3: Average heavy metal contents in mg per kg soil for Switzerland (from Keller & Desaules, 2001).

Land use	Cd [mg/kg]	Cu [mg/kg]	Zn [mg/kg]	Pb [mg/kg]	Ni [mg/kg]	Cr [mg/kg]	Hg [mg/kg]
Permanent grassland	0.309	18.3	64.6	24.6	22.3	24.0	0.088
Arable land	0.24	20.1	49.6	19.5	23.0	24.1	0.073
Horticultural crops	0.307	39.2	70.1	24.9	24.8	27.0	0.077

The original values for Switzerland are used as default (Tab. 21).

The balance of all inputs into the soil (fertilisers, pesticides, seed and deposition) and outputs from the soil (exported biomass, leaching and erosion), multiplied by the allocation factor is calculated as an emission to agricultural soil.

$M_{soil\ i} = (\Sigma\ inputs_i - \Sigma\ outputs_i) * A_i$

If the uptake of heavy metals by plants and the emissions from leaching and erosion exceed the inputs, a negative balance will result. This happens in particular if a large biomass is harvested and the inputs are low. The heavy metals are transferred to the biomass and have to be appropriately considered in the subsequent life cycle modelling (i.e. returned to the soil, transferred to the water or to landfills at the end of the life cycle).

A certain fraction of the heavy metal input into the soil stems from atmospheric deposition. The deposition would occur even without any agricultural production and is therefore not charged to the latter. An allocation factor accounts for this. The farmer is therefore responsible for a part of the inputs only (the rest stems mainly from other economic sectors), therefore only a part of the emissions is calculated in the inventory.

$$A_i = M_{agro\ i} / (M_{agro\ i} + M_{deposition\ i})$$

A_i allocation factor for the share of agricultural inputs in the total inputs for heavy metal i

$M_{agro\ i}$ total input of heavy metal from agricultural production in mg/(ha*year) (fertiliser + seeds + pesticides)

$M_{deposition\ i}$ total input of heavy metal from atmospheric deposition in mg/(ha*year) (Tab. 4)

In cases, where $M_{agro\ i} = 0$, i.e. no agricultural inputs to the soil occur, A_i also becomes 0.

Tab. 4: Heavy metal deposition (see Freiermuth 2006).

	Cd	Cu	Zn	Pb	Ni	Cr	Hg
Deposition [mg/ha/year]	700	2400	90400	18700	5475	3650	50

Tab. 5: Heavy-metal contents of plant material (mg/kg dry matter, from Freiermuth 2006).

Element	Cd	Cu	Zn	Pb	Ni	Cr	Hg
Unit	[mg/kg DM]						
Generic mean	0.10	6.6	32.0	0.54	1.04	0.55	0.04
Grass / Hay	0.13	8.6	40	1.2	1.68	1.09	0.15
Maize grains	0.03	2.5	21.5	0.3	1.16	0.32	0
Maize silage	0.1	5	34.5	1.61	0.48	0.7	0.01
Wheat grains	0.1	3.3	21.1	0.2	0.2	0.2	0.01
Wheat straw	0.2	2.5	9.6	0.6	0.6	0.7	NA
Barley grains	0.03	4.3	26.6	0.2	0.1	0.1	NA
Barley straw	0.1	4.8	11.1	0.6	0.8	1.2	NA
Rye straw	0.1	3.2	13	0.4	0.7	0.5	NA
Potatoes	0.04	6.45	15	0.55	0.33	0.57	0.09
Rape seed	1.6	3.3	48	5.25	2.6	0.5	0.1
Faba beans	0.04	6	30.1	0.87	1.3	0.69	0
Soya beans	0.06	15.1	47.7	0.08	5.32	0.52	0
Protein peas	0.09	10	73	0.16	0.83	0.32	0.01
Sugar beets	0.4	12	36.4	1.16	1.08	1.775	0.095
Rice grains	0.02	5.27	43.9	0.96	0.97	0.49	NA

Tab. 6: Heavy-metal contents of mineral fertilisers [mg/kg nutrient] according to Desaules & Studer (1993). No data available on Hg. Source: Freiermuth (2006).

Mineral fertilisers (%N/%P2O5/%K2O/%Mg)	Cd [mg/kg nutrient]	Cu [mg/kg nutrient]	Zn [mg/kg nutrient]	Pb [mg/kg nutrient]	Ni [mg/kg nutrient]	Cr [mg/kg nutrient]
Urea (46/0/0) kg N	0.11	13.04	95.65	2.39	4.35	4.35
Calcium ammonium nitrate (20/0/0) kg N	0.25	60.00	155.00	5.50	90.00	10.00
Ammonium nitrate (27.5/0/0) kg N	0.18	25.45	181.82	6.91	47.27	14.55
Ammonium sulphate (21/0/0) kg N	0.24	19.05	142.86	5.24	8.57	9.52
Calcium ammonium nitrate (27/0/0) kg N	0.19	8.52	100.00	5.93	12.59	2.96
Magnesium ammonium nitrate (23/0/0/5) kg N	0.43	56.52	4.35	4.35	21.74	6.09
Generic mean N	0.21	22.25	121.43	5.37	17.17	7.81
Triple superphosphate (0/46/0) kg P2O5	113.04	97.83	650.00	7.61	95.65	567.39
Superphosphate (0/19/0) kg P2O5	52.63	121.05	852.63	578.95	105.26	342.11
Thomas meal (0/16/0) kg P2O5	1.56	250.00	425.00	75.00	125.00	12212.50
Hyperphosphate/raw phosphate (0/26/0) kg P2O5	50.00	115.38	915.38	23.85	76.92	611.54
Generic mean P	51.32	118.22	751.32	49.42	100.46	589.46
Potassium chloride (KCl) (0/0/60) kg K2O	0.10	8.33	76.67	9.17	3.50	3.33
Potassium sulphate (0/0/50) kg K2O	0.10	4.00	64.00	6.60	1.60	4.00
Raw potassium (0/0/26/5) kg K2O	0.19	173.08	153.85	11.54	11.54	173.08
Lime kg CaO	0.12	4.00	8.00	3.60	12.20	314.00
Generic mean K	0.11	6.17	70.33	7.88	7.52	88.54

Tab. 7: Heavy-metal contents of farmyard manure and organic fertiliser (mg/kg DM, compiled by Freiermuth 2006 from from Menzi & Kessler (1998) and Desaules & Studer (1993, p. 152)). Dry matter (DM) contents from Walther et al. (2001, Tab. 44).

Farmyard manure	Cd	Cu	Zn	Pb	Ni	Cr	Hg	DM-content
Cattle liquid manure	0.18	37.1	162.2	3.77	4.3	3.9	0.4	9.0%
Cattle slurry	0.16	19.1	123.3	2.92	3.1	2.1	0.6	7.5%
Cattle staple manure	0.17	23.9	117.7	3.77	4.3	3.9	0.4	19.0%
Cattle manure form loose housing	0.15	22.0	91.1	2.81	4.3	3.9	0.4	21.0%
Pig liquid manure	0.21	115.3	746.5	1.76	8.6	6.7	0.8	5.0%
Pig solid manure	0.21	115.3	746.5	1.76	8.6	6.7	0.8	27.0%
Litter from broilers	0.29	43.8	349.2	2.92	40.0	10.0	0.2	65.0%
Litter from belts from laying hens	0.25	39.6	468.4	2.24	7.9	5.5	0.2	30.0%
Litter from deep pits from laying hens	0.25	39.6	468.4	2.24	7.9	5.5	0.2	45.0%

In some cases, the users want to exclude heavy metal uptake by the biomass from the total heavy metal flows. This can e.g. be the case if an incomplete life cycle is modelled. For this purpose the uptake by the crops is modelled in separate inventories (separated from the inputs). These datasets are called "product, uptake" (e.g. "wheat grains, uptake"). The heavy metal uptake is included as negative emissions into agricultural soil. A switch parameter "heavy_metal_uptake" is introduced allowing exclusion of heavy metal uptake in such situations.

2.8. Carbon dioxide (CO_2) emissions after urea or lime applications

After application of urea and lime, fossil CO_2 is released to the air. The worst-case approach according to IPCC (2006) is followed, so that the total amount of C is considered as released to the air is the form of CO_2.

For urea, the emission is 1.57 kg CO_2/kg Urea-N[3].

For limestone ($CaCO_3$) and dolomite ((Ca Mg)CO_3) the following emission factors apply:

- 12/100 * 44/12 = 0.44 kg CO_2/kg limestone
- 12/92.2 * 44/12 = 0.48 kg CO_2/kg dolomite.

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[3] The molecular weight of urea (CH4N2O) is 60, the C content is 12/60, the N content is 28/60, the conversion of C into CO_2 is 44/12, from which follows: 12/60*60/28*44/12=1.57.

2.9. Land transformation and occupation

2.9.1. Land transformation

2.9.1.1.　Definitions: direct and indirect land use change

Land transformation is a change from one land use type to another as a result of a human activity. The amount of land transformed is the area required to produce 1 functional unit of a product. Land use change has impacts on soil properties (e.g. carbon content, compaction, nutrients leaching, N_2O emissions among others), on biodiversity, on biotic production (Brandão and Milà i Canals 2012; Koellner *et al.* 2013; Koellner *et al.* 2012) and on other environmental aspects such as landscape, albedo and evapotranspiration (Spracklen *et al.* 2012).

Direct (dLUC) and indirect (iLUC) land use changes are often distinguished. Direct land use change can be defined as a change directly related to the history of the piece of land occupied. Indirect land use change can be defined as a change that appears in a different area than the direct land use as an indirect consequence. Typical example of iLUC is the increase of soybean production in Brazil that forces cattle production to move to other regions, where deforestation tends to increase as a consequence of increased pressure on land (Lapola *et al.* 2010). There is no international consensus on how to consistently and systematically address LUC in life cycle inventory, despite significant research in the LCA community (Bauen *et al.* 2010; Fritsche *et al.* 2010; Gnansounou *et al.* 2009; Nassar *et al.* 2011; Schmidt 2008; Searchinger *et al.* 2008; Sylvester-Bradley 2008; Tipper *et al.* 2009). Therefore, in the modelling here, no formal difference is made between dLUC and iLUC.

2.9.1.2.　Land use change from crop production

In crop production, global land transformation impacts are mainly driven by deforestation of primary forests. However, land use change from secondary forest or grassland to arable land must also be addressed in the inventory. Land use change from perennial to annual crops is also assessed.

LUC from crop production follows the methodology applied in ecoinvent V3.0 (Nemecek et al. 2014), which is based on IPCC (2006) methodology. The quantification of the land use change areas is based on annualized, retrospective data of the last 20 years. All carbon pools are considered for all of the vegetation categories affected (Tab. 8: Carbon pools accounting in land transformation

Carbon pool	Land transformation				
	From primary forest	From secondary forest	From perennial crop	From annual crop	From grassland
AGB [1]	8% harvested and stored 92% emitted (20% burned, 72% by decay)			100% emitted by decay Net carbon capture may occur in certain cases (and is taken into account)	
BGB [2]	100% emitted by decay				
DOM [3]	100% emitted by decay			Ignored	
SOC [4]	SOC change according to IPCC 2006, including peat drainage emissions. Net carbon capture may occur in certain cases (and is taken into account)				

(1) Aboveground biomass; (2) Belowground biomass; (3) Dead organic matter; (4) Soil organic carbon

In cases where the crop area in the country and its corresponding total land type area have increased in the considered time period, and if the area occupied by the natural ecosystem decreased during the same time period, the direct LUC is considered to be potentially relevant (Milà i Canals *et al.* 2012). Otherwise, LUC from a given land type is irrelevant to the life cycle inventory.

Two alternative approaches for allocating LUC are modelled. Both are country specific.

1. Crop-specific approach (default): land use change is allocated to all crops and activities that grew in the last 20 years in a given country, and only to them, according to their respective area increase. Crops which surface decreased are neither attributed any LUC impacts nor credits.

2. Shared-responsibility approach: land use change during the last 20 years is evenly distributed among all crops and activities present in the country, based on current area occupied.

For the default allocation, calculation of the area of land transformed per hectare of crop is computed with a Microsoft Excel tool[4] developed to support the estimates of LUC emissions based on the PAS2050-1/ENVIFOOD protocol approach. This tool uses has been developed by Blonk Consultants in 2013 and has been modified by Quantis to comply with WFLDB's requirements[5]. It uses statistical data for crops production and natural land areas in all countries from 1989 to 2012 (FAOSTAT 2012), as well as for country climates and soil types (EU-JRC 2010c). It has been reviewed and approved by the World Resources Institute (WRI) for use in the GHG Protocol.

To attribute LUC associated with the increase in area of each crop, a time period of 20 years is used for the calculation of the average annual increment. The same time period is applied for the amortisation of the emissions, which is aligned with PAS 2050-1 (BSI 2011a, BSI 2011b), FAO guidelines for feed supply chains (LEAP 2014) and ecoinvent V3.0 (Nemecek *et al.* 2014).

Four kinds of carbon pools – aboveground biomass (AGB), belowground biomass (BGB), dead organic matter (DOM) and soil organic carbon (SOC) – and four categories of vegetation – primary forest, secondary forest, grassland and perennial cropland – are considered. The values for the relevant carbon pools are taken from the IPCC Agriculture, Forestry and Other Land Use (AFOLU) report (IPCC 2006) and FAO (2010), Annex 3, Table 11.

For land transformation from primary forest and secondary forest, it is assumed that 20% of the AGB is burned and 8 % harvested (Houghton *et al.* 2000). The BGB, the DOM and the remaining slash from the AGB decay. In other words, 92% of carbon stored in AGB, and 100% of BGB and DOM are transferred into the atmosphere as biogenic CO_2. This approach is in line with the default (tier 1) assumptions of the IPCC (IPCC 2006).

For land transformation from grassland, no harvest or burning of biomass is considered. 100% of AGB and BGB carbon is transferred into the atmosphere as biogenic CO_2. DOM is considered negligible.

Land transformation from perennial to annual cropland is also accounted for, using the above-mentioned "Direct Land Use Change Assessment Tool".

For all categories of vegetation, change in SOC is accounted for in land occupation, since it is associated to the following land use category (section 2.9.2). SOC-related emissions from peat drainage are included (Joosten, 2010; IPCC, 2013)

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[4] "Direct Land Use Change Assessment Tool", version 2014-1-21-january-2014. Available for download at www.blonkconsultants.nl

[5] Latest edition is "WFLDB-adapted-Blonk 2014 direct-land-use-change-assessment-tool_2015-06-11a". Available upon request to Quantis. That version includes the following changes: SOC-related emissions include peat drainage emissions in the whole World, when occurring; suppression of the "set-to-zero" policy when carbon capture occurs; addition of more calculations and adaptation of the modelling structure for integration into the World Food LCA Database; correction of several crops definitions.

Losses of SOC are accompanied by mineralization of N, which in turn leads to emissions of N_2O. To determine the amount of N mineralization, the C:N ratio has to be known. IPCC (2006) gives a default value of 15 for the conversion of forest or grassland to cropland. For cropland the value of 11 is used (see **Erreur ! Source du renvoi introuvable.**). The emission factor for N_2O from mineralized N is 1 % (kg N2O-N/kg N) (IPCC, 2006, Tab. 11.1, EF1).

Tab. 8: Carbon pools accounting in land transformation

Carbon pool	Land transformation				
	From primary forest	From secondary forest	From perennial crop	From annual crop	From grassland
AGB [1]	8% harvested and stored 92% emitted (20% burned, 72% by decay)			100% emitted by decay Net carbon capture may occur in certain cases (and is taken into account)	
BGB [2]	100% emitted by decay				
DOM [3]	100% emitted by decay			Ignored	
SOC [4]	SOC change according to IPCC 2006, including peat drainage emissions. Net carbon capture may occur in certain cases (and is taken into account)				

(1) Aboveground biomass; (2) Belowground biomass; (3) Dead organic matter; (4) Soil organic carbon

2.9.2. Land occupation

2.9.2.1.   Definition

Measured in [m^2y], land occupation is calculated by multiplying the occupied area by time. Land occupation starts after the harvest of the previous crop (average harvest date) and ends with the harvest of the considered crop. If the date of the harvest of the previous crop is unknown, a period of 12 months is assumed, unless it is known that there is more than one cropping season per year. The previous crop is the last crop on the same field, where a physical product is harvested (previous main crop, catch crop for fodder or pasture) (Nemecek *et al.* 2011).

Impacts associated with land occupation result from changes in soil organic carbon (SOC) content, which results in the release of N_2O. The model is described in Nemecek *et al.* (2014) and is based on IPCC guidelines (2006).

2.9.2.2.   Land management change effects on soil carbon

Within the same land use category, changes in management can occur with consequences on SOC contents. This concerns e.g. if the tillage intensity on cropland is reduced (plough → reduced tillage → no-till) or if organic manure is added on cropland, where no organic fertiliser was previously applied. In grassland systems, SOC can be increased by improving the management. These changes in SOC are only accounted for if there is a permanent change in management according to IPCC (2006, Table 5.5 for cropland and Table 6.2 for grassland). Land management changes are considered in the same way as for land use changes. For cropland or grassland that is continuously managed in the same way (as it is e.g. the case for grassland and pasture without changes in management intensity), no change in SOC is calculated.

2.10.   Pesticide emissions

The amount of different active ingredients is entered by the user. This section describes the modelling of the pesticide emissions in the crop inventories.

In the ecoinvent database, pesticide emissions are modelled as 100% of the substance emitted to agricultural soil.

2.11.   Irrigation

The water amount for irrigation is given by the user. The tool maps this information with the corresponding irrigation datasets of ecoinvent. The origin of the groundwater as well as the proportion of the emissions of water to air, to groundwater and surface water are given by the ecoinvent report on irrigation (Laura Rubio et al. 2017).

2.12.   Carbon uptake by plants

Carbon is taken up in the form of carbon dioxide and fixed in the biomass. The carbon dioxide uptake by the growing crops is considered a resource input, which is important for the assessment of the climate change impact.

It is calculated from the carbon content of the products, which in turn can be calculated from the carbohydrate, protein, fat, fibre, and ash composition of the harvested products and the carbon contents (Nemecek & Kägi 2007, Tab. 21). The CO_2 uptake by the plant is estimated by multiplying the carbon content in the plant dry matter by the stoichiometric factor 44/12. Data on the composition of different products can be found e.g. in the USDA National Nutrient Database (http://ndb.nal.usda.gov/), Feedipedia (http://www.feedipedia.org/) or in the Swiss feed database (http://www.feed-alp.admin.ch). If no composition information is available, 47.5% is taken as default value for carbon content of dry mass (http://www.fao.org/forestry/17111/en/). If other sources than the above-mentioned are used, this will be described in the dataset-specific documentation. Carbon bound in crop residues that remain on the field is not considered as residues are decomposed and carbon is thus released.

The net release of biogenic CO_2 from biomass is included as 'Carbon dioxide, biogenic'. Only net changes of biomass stocks are considered, i.e. if the C stock in the biomass changes between the beginning and the end of the inventory period (typically a growing season).

Tab. 9: Carbon contents of different fractions of the biomass

Fraction	C-content (g/kg dry mass)	Source
Carbohydrates	440	Rouwenhorst et al. (1991)
Proteins	530	Rouwenhorst et al. (1991)
Lipids	750	Nemecek & Kägi (2007)
Fibres	440	Nemecek & Kägi (2007)
Ash	0	Nemecek & Kägi (2007)

3. References

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