Sphera’s Agricultural LCA model

Part 1

Model & Methods

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On behalf of Sphera Solutions, Inc., and its subsidiaries

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Abbreviations

The following overview of abbreviations is applicable to both documentations (Part 1 and Part 2).

General abbreviations

AFOLU	Agriculture, Forestry and Other Land Use
AWARE	Available Water Remaining
BNF	Biological Nitrogen Fixation
CCC	Crop Country Combinations
GIS	Geographical Information System
ILCD	International Reference Life Cycle Data System
KUE	Potassium Use Efficiency
LCA	Life Cycle Assessment
LCA FE	Life Cycle Assessment for Experts (formerly known as 'GaBi ts') Software
LCI	Life Cycle Inventory
LANCA®	Land Use Indicator Value Calculation in Life Cycle Assessment
LUC	Land Use Change
LULUC	Land Use and Land Use Change
MLC	Managed LCA Content, by Sphera (formerly known as 'GaBi ts databases')
NUE	Nitrogen Use Efficiency
PAS	Publicly Available Specifications
PEF	Product Environmental Footprint
PUE	Phosphorous Use Efficiency
SALCA	Swiss Agricultural Life Cycle Assessment

Organizational Units

AquaStat	FAO global information system on water resources and agricultural water management
ECN	European Competition Network of the European Commission
ESDAC	European Soil Data Centre
FAO	Food and Agriculture Organization of the United Nations
FAOStat	FAO global information system on food and agricultural data
IFA	International Fertilizer Association
IPCC	Intergovernmental Panel on Climate Change
ISO	International Organization for Standardization
JRC	Joint Research Centre of the European Commission
KTBL	Kuratorium für Technik und Bauwesen in der Landwirtschaft
NRCS	National Resources Conservation Service of the USDA
OECD	Organization for Economic Cooperation and Development
USDA	United States Department of Agriculture
WULCA	Working group on the assessment of Use and depletion of water within LCA

Emissions

EF	Emission Factor
GHG	Greenhouse Gas
CH_4	Methane
CO_2	Carbon Dioxide
N_2O	Nitrous Oxide
NH_3	Ammonia
NO_2	Nitrogen Dioxide
NO_x	Nitric Oxides
SO_2	Sulphur Dioxide

Fertilizers

AN	Ammonium Nitrate
$CaCO_3$	Calcium Carbonate
CaO	Quicklime
DAP	Diammonium Phosphate
H_3PO_4	Phosphoric Acid
KCl	Potassium Chloride
MAP	Monoammonium Phosphate
NH_3	Ammonia
NPK	Nitrogen Phosphate Potassium
RP	Rock Phosphate
TSP	Triple Superphosphate
UAN	Urea Ammonium Nitrate

Elements

As	Arsenic
Cd	Cadmium
Cr	Chromium
Cu	Copper
Hg	Mercury
K	Potassium
K_2O	Potassium Oxide (typically listed as K in fertilizers)
N	Nitrogen
Ni	Nickel
P	Phosphorous
Pb	Lead
P_2O_5	Phosphate
Tl	Thallium
U	Uranium
Zn	Zinc

1. Introduction

Sphera's Agricultural LCA Model has been developed to assess the environmental impacts of crop cultivation from cradle to field gate using the most recent LCA-centred methodology for representing agricultural production systems. It is a robust and tested model, based on agreed standards for agricultural modelling in LCA that has been further developed from the first comprehensive and industry-leading model of 2003. The two current, main guiding standards for Agricultural modelling are:

- 2019 Refinement of the IPCC Guidelines for National Greenhouse Gas Inventories (IPCC, 2019)
- Product Environmental Footprint method (European Commission, 2021)

Another relevant guideline in this context is the GHG Protocol Land Sector and Removals Guidance Draft (GHG Protocol, 2022). The model was examined in relation to this guideline and no deviations were identified. The GHG Protocol Guidance primality references the IPCC guidelines. The finalized version of the guidance remains to be published (expected in 2024).

Sphera's Agricultural LCA Model is a generic model that can be used by generally experienced LCA practitioners with and without in-depth agricultural expertise (e.g. for screening studies or scope 3 emission modelling). The model is intended to work with data that is readily available (i.e. data that can be retrieved from secondary sources or collected with reasonable effort as primary data) to conduct agricultural LCI and LCA studies. It is created with the LCA FE (LCA for Experts, formerly known as "GaBi ts") software system for life cycle engineering. It represents the basis for Sphera's own agricultural datasets, providing high quality LCI data following a consistent and scientific approach, included in the Sphera MLC background database.

The goal of this document is to provide the relevant background information on Sphera's Agricultural LCA Model. The methodology and data applied to create datasets is described in the second part of the documentation (Part 2: Dataset Generation & Data Sources). The present document organization is summarized below:

- Chapter 1: Introduction to Sphera's Agricultural LCA Model
- Chapter 2: Description of Sphera's Agricultural LCA Model
- Chapter 3: Emission modelling in Sphera's Agricultural LCA Model

2. Sphera's Agricultural LCA Model

The following sections describe the general scope of Sphera's Agricultural LCA Model. This includes, but is not limited to, the description of the functional unit, the system boundaries as well as information about the software and databases used.

2.1. Product System and Functional Unit

The function of the product system is an open field cultivation of agricultural crops. Both perennial and annual crop cultivation systems can be assessed using this model.

The default functional unit is defined as:

Production of 1 kg agricultural crop at field gate.

In addition, the model offers three possible functional units that can be selected. Those are:

- 1 kg agricultural crop at field gate
- 1 tonne agricultural crop at field gate
- production of crop on 1 hectare land area at field gate

Co-products taken off the field (e.g. straw) can be considered and allocation applied, see section 2.3.

2.2. System Boundary

The system boundary of the model represents the crop production from cradle to farm gate. To a certain extent, the system boundary is flexible for further adjustments according to the needs of the client or the LCA practitioner. The following table provides aspects of the default system boundary used in the Agricultural LCA model.

Table 2-1: Overview of system boundaries

Included	Excluded
✓ Fertilizer and pesticide production ✓ Irrigation and related energy consumption ✓ Transports ✓ Seed and planting material inputs ✓ Field emissions ✓ Emissions from fertilizer and pesticide application ✓ Field clearing, biomass burning ✓ Land use change emissions (if applicable, can be assessed separately) ✓ Methane emissions from flooded rice cultivation ✓ Emissions from soil erosion ✓ Uptake of heavy metals into crops (optional)	× Capital goods × Animal draught × Human labour

All material and energy flows required for the cultivation are included, as well as all associated wastes and emissions. This includes but is not limited to: fertilizer and pesticide production as well as field emissions (e.g. N_2O), emissions related to fire clearing (i.e. the combustion of biomass remaining on the field from previous cultivation period) (e.g. CH_4, SO_2), electricity and all transports.

Environmental impacts associated with draught animals as well as construction of capital equipment and maintenance of support equipment are excluded as they usually only show minimal contribution. However, if these aspects should be considered, additional modules can be added to the model. Social aspects are beyond the scope of the model and therefore, human labour is also excluded.

2.3. Allocation

The model provides different options to conduct allocation based on energy content, carbon content, nitrogen content, mass or prices. The product characteristics used for allocation need to be specified before.

2.4. Overview of Model Modules

The model is structured into different modules, as displayed in Table 2-2, which can also be used to structure the results at the end. Thereby, each module or subprocess can be evaluated separately using the grouping function of the LCA FE software to conduct a contribution analysis.

Table 2-2: Overview of model modules and approaches

Module	Description	Approach
Provision of fertilizer	Emissions and resource flows related to fertilizer production	(see below)
Fertilizer production	Upstream emissions and resource flows in the fertilizer supply chain (e.g. energy consumption of production)	Based on fertilizer production datasets from Sphera MLC database
Irrigation	Emissions and resource flows from water irrigation	(see below)
Irrigation water requirement	Water used for irrigation	Based on collected data
Irrigation energy	Energy consumption from pumps, includes impacts of provision of energy and combustion emissions and resource flows (in case of diesel pumps)	Can be specified or estimated based on pump model in Sphera MLCdatabase
Transports	Transports of agricultural inputs (fertilizer and pesticides to the field	Based on transport distance, using the truck model in Sphera MLC and provision of diesel
Field emissions	Emissions from agricultural soil related to fertilizer application, crop residues and soil erosion	(see below)
Emissions from fertilizer application (direct and indirect field emissions)	Nitrous oxide emissions to air from microbial nutrient turnover (denitrification), ammonia emissions to air from mineral and organic fertilizer, nitrate emissions to water through leaching, carbon dioxide emissions from carbon contained in fertilizer (urea, lime)	Based on approach and emission factors provided in 2019 IPCC guidelines; fuel consumption considered under field work

Emissions from crop residues	Additional nitrogenous emissions due to nitrogen contained in crop residues	Based on approach provided in 2019 IPCC guidelines
Emissions from soil erosion	Nutrients contained in the soil reaching surface water bodies with soil erosion	Can be specified or estimated based on data from Global Soil Erosion Modelling platform (GloSEM) and default nutrient content in soil
Field Clearance	**Emissions related to the combustion of biomass after cultivation to clear the field**	**(see below)**
Emissions from combustion of biomass	Methane, ammonia, nitrous oxide and other emissions related to the combustion process	Modelled based on the amount of biomass burned, its carbon and nitrogen content, based on emission factors from (Battye & Battye, 2002).
Field work	**Emissions from tractor use and provision of fuel**	**(see below)**
Tractor use	Emissions from fuel combustion	Based on tractor and truck model in Sphera MLC
Provision of Diesel	Upstream emissions **and resource flows** in the fuel supply chain (e.g. refinery)	Based on energy provision datasets from Sphera MLCdatabase (yearly updated)
Crop protection	**Emissions and resource flows related to production and application of crop protection agents**	**(see below)**
Pesticide production	Upstream emissions **and resource flows** in the pesticide supply chain (e.g. energy consumption of production)	Based on pesticide production datasets from Sphera MLC database
Pesticide application	Emission of pesticides into the environment	Generic emission factors to air, water and soil used according to PEF method (90% to soil, 9% to air, 1% to water). Latest default method from PEF method recommended for toxicity assessment (Dec 2021).
Emissions from LULUC	Carbon dioxide emissions related to the conversion of forest (or other land use type) to agricultural land.	Based on primary data and FAO statistical data using approach from PAS 2050

2.5. Software, Database and Background Data

The LCA model was created using the Sphera LCA FE Software system for life cycle engineering. The Sphera MLC2023 LCI database provides the life cycle inventory data for several of the raw and process materials obtained from the background system. For reference, the background data in Sphera MLC was used, the complete list of all datasets used is provided in Annex 4 – Overview on background datasets. Complete documentation for each of the datasets can be found online at https://sphera.com/product-sustainability-gabi-data-search/.

2.6. Required Input Data

Users of the model should have the following input data available:

- Yield
- Seed input
- Total N, P, K inputs and fertilizer type
- Water and energy used for irrigation
- Pesticide use
- Machinery use and fuel consumption
- Land use change (land use in the last 20 years)
- Fraction of farmers applying field clearance

Secondary data or Sphera's Managed LCA Content (MLC) databases (former "GaBi Databases") can be used to consistently fill data gaps if necessary, and add any additional processes and consumables, following the procedures developed by Sphera to create the agricultural datasets in the MLC (see also document Part 2: Dataset Generation & Data Sources).

3. Emission Modelling

The following chapter provides an overview of all emission modelling specifications as integrated in Sphera's Agricultural LCA Model. In general, the IPCC guideline is the most used guideline for emission modelling. However, each subchapter provides the specific sources on which the respective emission modelling is based on. While the model automatically includes default values, all emission factors can be individually adjusted for other use cases, e.g. different spatial resolutions for regionalization or for comparability to reference studies.

3.1. Field Emissions

Included in the definition of field emissions, as described in this section, are emissions from agricultural soils to air and water. Those are mainly related to fertilizer application, crop residues as well as soil erosion. This chapter also provides details on heavy metals, methane emissions and emissions from changes in soil carbon stocks.

3.1.1. Fertilizer Application

The application of fertilizer causes direct and indirect field emissions, which are subdivided as follows:

- Nitrous oxide (N_2O) emissions to air from microbial nutrient turnover (denitrification)
- Ammonia (NH_3) emissions to air from mineral or organic fertilizer
- Nitrate (NO_x) emissions to water through leaching
- Carbon dioxide (CO_2) emissions from carbon contained in fertilizer (urea, lime)

The emission modelling is based on the IPCC guideline and their respective emission factors (IPCC, 2019). As stated before, those emission factors can be adjusted in the model. The table below provides the available default values from the IPCC:

Table 3-1: IPCC emission factors of fertilizer application

EF	Aggregated	Disaggregated		Unit
EF N_2O	0.010	Synthetic fertiliser inputs in wet climates	0.016	[kg N_2O-N/kg N applied]
		Other N inputs in wet climates	0.006	
		All N inputs in dry climates	0.005	
EF NH_3 synthetic	0.011	Urea	0.15	[kg NH_3-N/kg N applied]
		Ammonium-based	0.08	
		Nitrate-based	0.01	
		Ammonium-Nitrate-based	0.05	
EF NH_3 organic	0.21	-	-	-
EF NO_3-N	0.24	Only applicable in wet climates		

Additionally, an alternative approach to model nitrate emissions is available in the model. The IPCC provides a default emission factor for nitrate emissions, 24% of the nitrogen applied is being lost as emissions via leaching. This value represents a rough estimate and can lead to unrealisticalle missions. As an example, systems that are running on low N-input and still report high yields might drain nitrogen from the soil which would need to be replaced later, or such systems could not be maintained over long periods of time. A simple default value can also lead to unrealistically low emission results for crops that receive a substantial surplus (e.g. for some vegetables and annual fruit crops). In any case, the approach will lead to a nitrogen balance that is not closed (emissions + uptake > input). Therefore, Sphera's Agricultural LCA Model can optionally consider the recommended N-Balance approach as documented in the PEF method (European Commission, 2021):

- <u>In case of a nitrogen surplus in the soil:</u>
  the surplus of nitrogen is assumed to be lost via nitrate leaching
- <u>In case of a nitrogen deficit:</u>
  the missing nitrogen is inventoried as additional fertilizer input (incl. related emissions)[1]

The details of the N-Balance approach are provided in Annex 1.

3.1.2. Crop Residues

This section describes emissions occurring due to the decomposition of crop residues. The emissions are modelled according to the IPCC Guidelines (IPCC, 2019). All details can be found in table 11.1A in the 2019 Guidelines, as displayed in Figure 3-1. The table includes parameters such as dry matter fraction, nitrogen content of above and below-ground crop residues as well as the ratio of the residues to the yield. Only the emissions of the current crop are considered. No emissions from the previous crops are included in the calculations.

[1] An additional argument to equal out a nitrogen deficit is that this is expected to occur in real practice, where additional nitrogen might be applied the following crop, compensating for the loss of N from the previous crop.

Crops	N content of above-ground residues ($N_{AG(T)}$)[a]	N content of below-ground residues ($N_{BG(T)}$)[a]	Ratio of above-ground residue dry matter to harvested yield ($R_{AG(T)}$)[b]	Ratio of below-ground biomass to above-ground biomass ($RS_{(T)}$)[a]	Dry matter fraction of harvested product (DRY)[a]
TABLE 11.1A (NEW) DEFAULT VALUES FOR $N_{AG(T)}$, $N_{BG(T)}$, $R_{AG(T)}$, $RS_{(T)}$ AND DRY TO BE USED IN EQUATIONS 11.6 AND 11.7					
Crops					
Generic value for crops not indicated below[c]	0.008 (± 75%)[d]	0.009 (± 75%)[d]	1.0	0.22	0.85
Generic Grains	0.006 (± 75%)[d]	0.009 (± 75%)[d]	1.3	0.22 (±16%)	0.88
Winter Wheat	0.006 (± 75%)[d]	0.009 (± 75%)[d]	1.3	0.23 (±41%)	0.89
Spring Wheat	0.006 (± 75%)[d]	0.009 (± 75%)[d]	1.3	0.28 (±26%)	0.89
Barley	0.007 (± 75%)[d]	0.014 (± 75%)[d]	1.2	0.22 (± 33%)	0.89
Oats	0.007 (± 75%)[d]	0.008 (± 75%)[d]	1.3	0.25 (± 120%)	0.89
Maize	0.006 (± 75%)[d]	0.007 (± 75%)[d]	1.0	0.22 (± 26%)	0.87
Rye	0.005 (± 75%)[d]	0.011 (± 75%)[d]	1.6	-[e]	0.88
Rice	0.007 (± 75%)[d]	-[e]	1.4	0.16 (± 35%)	0.89
Millet	0.007 (± 75%)[d]	-[e]	1.4	-[e]	0.90
Sorghum	0.007 (± 75%)[d]	0.006 (± 75%)[d]	1.4	-[e]	0.89
Beans and Pulses	0.008 (± 75%)[d]	0.008 (± 75%)[d]	2.1	0.19 (± 45%)	0.91
Soybeans	0.008 (± 75%)[d]	0.008 (± 75%)[d]	2.1	0.19 (± 45%)	0.91
Potatoes and Tubers	0.019 (± 75%)[d]	0.014 (± 75%)[d]	0.4	0.20 (± 50%)[f]	0.22
Peanuts	0.016 (± 75%)[d]	-[e]	1.0	-[e]	0.94

Figure 3-1: Table 11.1A (New) from the IPCC Guidelines 2019

3.1.3. Soil Erosion

There are two important aspects to consider when looking at emissions from soil erosion: the amount of soil that is being eroded in the considered system as well as the nutrient contents and the corresponding emission factors. The amount of soil eroded can be entered based on primary or secondary data. Proxy values for soil erosion can be retrieved from the Global Soil Erosion Modelling Platform provided by the Joint Research Centre of the European Commission (ESDAC, 2019) (see also Part 2: Dataset Generation & Data Sources), and from the LANCA model (see section 3.4).

After obtaining the information, the amount of soil eroded is then multiplied with the nutrient contents of the soil, leading to emissions through nutrients contained in the soil reaching the surface water bodies via soil erosion. Note that only the amount of soil erosion reaching surface water bodies should be considered, the default value is 20% of total soil erosion (Prasuhn, 2006). The values for the nutrient and heavy metal contents of the top soil are based on (Tóth, Hermann, Szatmári, & Pásztor, 2016). The nutrient contents are listed in Table 3-2.

Table 3-2: Nutrient contents of top soil used for soil erosion emissions

Name of nutrient	Amount of nutrient	Unit as used in model
Arsenic	3.72	mg/kg content of topsoil
Cadmium	0.09	mg/kg content of topsoil

Chrome	6.35	mg/kg content of topsoil
Cobalt	21.7	mg/kg content of topsoil
Copper	13	mg/kg content of topsoil
Manganese	373	mg/kg content of topsoil
Mercury	0.04	mg/kg content of topsoil
Nickel	18.4	mg/kg content of topsoil
Organic carbon	0.01	kg/kg content of topsoil
Phosphate	0.001767	kg/kg content of topsoil

3.1.4. Phosphorous

Phosphorous emissions are not included in the IPCC Guidelines since they do not contribute to the climate change impact category. However, Phosphorous emissions are relevant for eutrophication. Relevant pathways for phosphorous emissions are the following:

- Soil erosion
- Run-Off
- Leaching

The approach to model emissions from soil erosion is described in the previous chapter. Run-off and leaching are based on default values derived from the SALCA-P model (D. Brockmann et al., 2014), providing the following average values:

- 0.00048 kg P/kg P_2O_5 for mineral fertilizer
- 0.00184 kg P/kg P_2O_5 for liquid organic fertilizer
- 0.00096 kg P/kg P_2O_5 for solid organic fertilizer

3.1.5. Heavy Metals

The emissions of heavy metals are relevant if the toxicity impacts of the product system are assessed. Emissions of heavy metals occur with soil erosion (see section 3.1.3) and through application of fertilizer. Both mineral and organic fertilizers contain heavy metals . The average heavy metal contents of organic and mineral fertilizers is taken from (Dittrich & Klose, 2008) and (Washington State Department of Agriculture, 2009), both are provided in Annex 2 – Fertilizer Product Characteristics.

Plant uptake of heavy metals should be considered in the model, if further life cycle models consider the related emissions (e.g. through biomass incineration etc.) If this is not the case, the uptake can be ignored (assumed to be zero). These approaches are described in the PEF method (European Commission, 2021).

3.1.6. Methane Emissions (from flooded rice cultivation)

The flooding of the soil for paddy rice cultivation leads to the release of methane emissions due to the anaerobic conditions. Sphera's Agricultural LCA Model provides two options to consider these emissions:

- Cultivation modelling according to Volume 4, Chapter 5.5 of the IPCC Guidelines (IPCC, 2019), the model uses the same parameters and equations as provided in the guideline
- Using the FAOStat values for rice methane emissions (FAOStat, 2022)

3.1.7. Emissions from Soil Organic Carbon Stock Changes

Emissions from soil organic carbon stock changes can optionally be included based on the IPCC Tier 1 method for soil organic carbon, as found in the IPCC guidelines. The model uses the same parameters and equations as provided in the IPCC guidelines.

3.2. Active Ingredient Application

While the production and provision of active ingredients (i.e. pesticides, herbicides and insecticides) usually have less relevant albeit not negligible impacts, the emissions resulting from the application have a high relevance for toxicity assessments. The emissions are based on a combination of the application rate (amount of active ingredient applied) and emission factors, which specify the fractions of the amount applied reaching air, water and soil compartments. For these emissions the default emission factors from the PEF method have been applied (European Commission, 2021):

- Emissions to soil: 90%
- Emissions to air: 9%
- Emissions to water: 1%

Those emission factors can be adjusted in the model, as also foreseen under the PEF Method, if data is available. For impact assessment, it is recommended to use the latest version of the toxicity factors provided in the Environmental Footprint method (i.e. EF 3.1; EF 3.0 has been superseeded and shall not be used anymore), while other methods are supported by the inventory. All active ingredients that can be selected in the model are characterized for the PEF method, a list is provided in the Annex.

3.3. Field Clearance

The term field clearance describes the process of biomass combustion after the cultivation in order to clear the field (if applicable). The emission factors in Sphera's Agricultural LCA Model approach are based on (Battye & Battye, 2002). The user needs to define the total amount of biomass combusted as well as the carbon and nitrogen content of the combusted biomass. The modul can also be applied to assess emissions from slash and burn clearing when a land use change occurs. .

3.4. Land Use (LANCA®)

Sphera's Agricultural LCA Model has implemented the LANCA® characterization factors (version 2022.1) for land use. Inventory data on crop and country specific land use are defined on the foreground system using the ILCD/EF land use flows for "occupation," "transformation to" and "transformation from". However, country and land use type (irrigated, non-irrigated, extensive, intensive etc.) need to be defined in the model. The LANCA® impact categories of erosion resistance, mechanical filtration, physicochemical filtration, groundwater regeneration and biotic production are included. For further information, please also refer to the official documentation: "Land Use LCI Modelling & Assessments 2024"[2].

3.5. Land Use Change

Sphera's Agricultural LCA Model does not directly model land use change emissions, but requires data input from an assessment outside of the model. For direct land use change (dLUC) data primary data (e.g. project data) is required. In case such primary data is not available or its traceability is limited, the model can consider statistical land use change (sLUC) as proxy in combination with Sphera's LUC Tool. This tool is following the recommendations of the European Commission and is therefore using the PAS 2050:2011

[2] http://www.gabi-software.com/fileadmin/Documents/Land Use LCI Modelling & Assessments 2024

and PAS 2050-1:2012 guidelines as basis. For details on the sLUC calculation conducted by Sphera, please refer to the second part of this documentation (Part 2: Dataset Generation & Data Sources).

3.6. Emission Modelling based on MLC Background Datasets

Some emissions considered in the model are based on background datasets from the Sphera MLC database. Those are listed below:

Table 3-3: Overview of emissions based on MLC background datasets

Module	Description	Approach
Fertilizer production and fertilizer provision	Upstream emissions and resource flows in the fertilizer supply chain (e.g. energy consumption of production)	Based on fertilizer production datasets from MLC database
Pesticide production	Upstream emissions and resource flows in the pesticide supply chain (e.g. energy consumption of production)	Based on pesticide production datasets from MLC database
Irrigation energy	Energy consumption from pumps, includes impacts of provision of energy and combustion emissions (in case of diesel pumps) and resource flows	Based on pump model in MLC
Transports	Transports of agricultural inputs (fertilizer and pesticides to the field	Based on transport distance, using the truck model in MLCand provision of diesel
Tractor use	Emissions from fuel combustion	Based on tractor and truck model in MLC
Provision of Diesel	Upstream emissions and resource flows in the fuel supply chain (e.g. refinery)	Based on energy provision datasets from MLC database (yearly updated)

The complete list of all datasets used is provided in Annex 4.

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Annex 1 – N-Balance Approach

The following section has been transferred from page L 471/236 of the PEF method (European Commission, 2021) in order to describe the N-Balance approach in more detail:

The N-balance is calculated using the parameters in Table 4 and the formula below. The total NO_3^-N emission to water is considered a variable and its total inventory shall be calculated as:

'Total NO_3^-N emission to water' = 'NO_3^- base loss' + 'additional NO_3^-N emissions to water', with

'Additional NO_3^-N emissions to water' = 'N input with all fertilisers' + 'N_2 fixation by crop' – 'N-removal with the harvest' – 'NH_3 emissions to air' – 'N_2O emissions to air' – 'N_2 emissions to air' -'NO_3^- base loss'.

If, in certain low-input schemes, the value for 'additional NO_3-N emissions to water' becomes negative, the value shall be set to '0'. Moreover, in such cases the absolute value of the calculated 'additional NO_3-N emissions to water' is to be inventoried as additional N-fertiliser input into the system, using the same combination of N-fertilisers as employed for the analysed crop.

This last step serves to avoid fertility-depletion schemes by capturing the N-depletion by the analysed crop that is assumed to lead to the need for additional fertiliser later on and to keep the same soil fertility level.

Table 4 Alternative approach to nitrogen modelling

Emission	Compartment	Value to be applied
NO_3^- base loss (synthetic fertiliser and manure)	Water	kg NO_3^-= kg N*FracLEACH = 1*0.1*(62/14) = 0.44 kg NO_3^-/ kg N applied
N_2O (synthetic fertiliser and manure; direct and indirect)	Air	0.022 kg N_2O/ kg N fertiliser applied
NH_3 - Urea (synthetic fertiliser)	Air	kg NH_3= kg N * FracGASF= 1*0.15* (17/14)= 0.18 kg NH_3/ kg N fertiliser applied
NH_3 - Ammonium nitrate (synthetic fertiliser)	Air	kg NH_3= kg N * FracGASF= 1*0.1* (17/14)= 0.12 kg NH_3/ kg N fertiliser applied
NH_3 - others (synthetic fertiliser)	Air	kg NH_3= kg N * FracGASF= 1*0.02* (17/14)= 0.024 kg NH_3/ kg N fertiliser applied
NH_3 (manure)	Air	kg NH_3= kg N*FracGASF= 1*0.2* (17/14)= 0.24 kg NH_3/ kg N manure applied
N_2-fixation by crop		For crops with symbiotic N_2-fixation: the fixed amount is assumed to be identical to the N-content in the harvested crop
N_2	Air	0.09 kg N_2 / kg N applied

Figure apx 1: Table 4 from PEF method (European Commission, 2021)

Annex 2 – Fertilizer Product Characteristics

The following table provides an overview of the fertilizer characteristics as used in Sphera's agricultural model. The average heavy metal contents of organic and mineral fertilizers are taken from (Dittrich & Klose, 2008) and (Washington State Department of Agriculture, 2009).

Table apx 1: Fertilizer product characteristics

Content	AN	Urea	NPK	CAN	NH_3	UAN	MAP	TSP	H_3PO_4	RP	KCl	$CaCO_3$	CaO	DAP	Unit
N	0.335	0.46	0.15	0.27	0.82	0.3	0.11	0	0	0	0	0	0	0.18	[kg N/kg] Nitrogen content of fertilizer
P_2O_5	0	0	0.15	0	0	0	0.52	0.46	0.54	0.324	0	0	0	0.46	[kg P_2O_5/kg] Phosphate content of fertilizer
As	0.43	0.09	1.3	0.35	0.5	0.26	6.04	6.24	6.24	3.96	0.49	2.94	2.48	7.97	[mg/kg] As content of fertilizer
Cd	0.05	0.01	0.73	0.05	0.02	0.03	9.24	28.26	28.26	11.69	0.01	0.07	0.69	19.91	[mg/kg] Cd content of fertilizer
Cr	4.4	0.61	13.2	0.88	1.41	2.51	144	229	229	118	0.58	6.53	787.93	272	[mg/kg] Cr content of fertilizer
Cu	7.1	0.83	7.21	1.47	2.32	3.97	23.8	15.3	15.3	5.37	0.74	1.56	0.04	26.5	[mg/kg] Cu content of fertilizer
Hg	23	0.01	0.01	0.01	2.31	11.51	0.03	0.02	0.02	0.02	0.01	0.23	0.01	0.01	[mg/kg] Hg content of fertilizer
Ni	13	0.27	0.97	0.03	4.74	6.64	19.5	20.9	20.9	3.81	0.62	10.46	3.22	35.1	[mg/kg] Ni content of fertilizer
Pb	1.9	0.35	2.55	21.1	2.4	1.13	3.69	14.7	14.7	3.82	0.29	18.44	2.21	0.87	[mg/kg] Pb content of fertilizer
Tl	0	0.02	0.05	0.02	0.38	0.01	0.18	0.35	0.35	1.2	0.07	0.02	0.01	0.31	[mg/kg] Tl content of fertilizer
U	0	0.01	5.58	0.36	0.11	0.01	76.7	104	104	22.5	0.03	2.41	14.1	121	[mg/kg] U content of fertilizer
Zn	50	3.67	69.4	40.9	17.67	26.84	191	354	354	154	2.26	75.93	93.35	330	[mg/kg] Zn content of fertilizer

Annex 3 – Active Ingredients

The table below provide a list of all active ingredients, which are available in the model as elementary flows by standard. Further active ingredients can be added depending on the scope of the assessment.

Table apx 2: List of available standard active ingredients in Sphera's agricultural model

2,4,5-Trichlorophenoxyacetic	Copperoxychlorid	Fentinhydroxid
2,4-Dichlorophenoxyacetic	Copper	Fenvalerate
2,4-DB	Cyanazine	Fipronil
ACEPHATE	Cyclanilide	Fluazinam
Acetamiprid	CYFLUTHRIN	Flumioazin
Acetochlor	CYPERMETHRIN	Fluometuron
Acifluorfen	Cyprodinil	Fluroxypyr
alpha-Hexachloro	Cyromazine	Flutolanil
Alachlor	DDT	Folpet
Aldicarb	Decan-1-ol	Fomesafen
Aldrin	DEF	Formothion
Aminopyralid	Deltamethrin	Glyphosate-isopropylammonium
Anilazine	Demeton	Glyphosat
Atrazine	Desmetrin	Halosulfuron-methyl
AVERMECTIN	Diazinon	Heptachlor

Azadirachtin	Dicamba	Heptenophos
Azinphos-ethyl	Dichlorprop	Hexazinone
AZODRIN	Dichlorvos	Imazethapyr
Azoxystrobin	Dicofol	IMIDACLOPRID
Azinphos	DICROTOPHOS	Ioxynil
Barban	Dieldrin	Iprodione
Benomyl	Diflufenican	Isoproturon
Bensulide	Dimethenamid	Isoxaflutole
Bentazon	Dimethoate	LAMBDA-CYHALOTHRIN
Bifenthrin	2,4-D,	Lindane
Bromoxynil	Dinoseb	Linuron
Calcium	Dinoterb	Malathion
Calcium	Diquat-dibromide	Mancozeb
Captafol	Disulfothon	Maneb
Captan	Diuron	MCPA
Carbaryl	DNOC	Mecarbam
Carbendazim	DP-MP063	Mecoprop
Carbofuran	Endosulfan	Mepiquat
Carfentrazone-ethyl	Endothall	Mesotrione
Chlormequat-chloride	Endrin	Metamitron
Chloropicrin	Dipropylthiocarbamic	Metam
Chlordane	Esfenvalerate	Metam

Chlorfenvinfos
Chloridazon
Chlormephos
Chloropyrifos
Chlorothalonil
Chlorpropham
Clomazone
Clopyralid
Coumaphos
Copper
Monolinuron
Morpholine
MSMA
Naled
Novaluron
Oxamyl
Oxydemeton-methyl
Oxyfluorfen
Paraffin
Paraquat
Parathion
Methyl

Ethalfluralin
Ethephon
Ethion
Ethoprophos
Etofenprox
Etoxazole
Fenitrothion
Fenthion
Fentin
Picloram
Pirimiphos-methyl
Pirimicarb
PROFENOFOS
PROMETRYNE
Propargite
Propanil
Propiconazole
Propachlor
Propoxur
Pymetrozine
Pyraflufen-ethyl
Pyrazophos

Metazachlor
Methyl
Methabenzthiazuron
Methomyl
Metobromuron
Metolachlor
Metribuzin
Metsulfuron-methyl
Mevinphos
Monocarbamide
Terbufos
Thiamethoxam
THIDIAZURON
Thifensulfuron
Thiobencarb
Thiodicarb
Thiophanate-methyl
Thiram
Tolclophos-methyl
Triallate
Triasulfuron
TRIAZOPHOS

PENDIMETHALIN

Permethrin

Phenthoate

Phorate

Phosalone

Phosmet

Phosphamidon

Phoxim

Pyrithiobac-sodium

Quinclorac

Quinalphos

Quinclorac

Simazine

S-Metolachlor

Tribenuron

Tributyltinoxide

Trichlorfon

Triclopyr

Trifluralin

Triflusulfuron-methyl

Zineb

Ziram

Annex 4 – Overview on background datasets

The following table provides an overview on background datasets as used in Sphera's Agricultural LCA Model. The complete documentation for each of the datasets can be found online at https://sphera.com/product-sustainability-gabi-data-search/.

Table apx 3: Overview background datasets used in Sphera's Agricultural Model

Nation	Name	Type	Source	Object	GUID
GLO	Truck, Euro 0 - 6 mix, 14 - 20t gross weight / 11,4t payload capacity	u-so	Sphera	Diesel	{70e7f7b6-666e-48ef-8b29-db8af48018ca}
GLO	Irrigation pump generic	u-so	Sphera	Field technique	{c0534d74-5cd8-4b07-9d58-c6153a4d4905}
GLO	Crop protection fate	u-so	Sphera	Field technique	{099f2197-dbd6-4933-8684-977d11171826}
GLO	Universal Tractor	u-so	Sphera	Field technique	{32775673-a2ad-46f8-a16e-9adff55297ea}
GLO	Biomass combustion (field)	u-so	Sphera	Field technique	{6b3401b2-efa2-4a88-bb4a-fddd385dd49d}
GLO	Pesticide (average)	agg	Sphera	Pesticides	{e2ae08d0-05cf-4b2a-a334-e8b42b796b3d}
US	Ammonium nitrate (AN, solid)	agg	Sphera	Fertilisers	{b9de2c53-5b7f-45c2-9241-18bcab357fe7}
US	Urea (agrarian)	agg	Sphera	Fertilisers	{a034a4cb-5091-489a-952c-ec34c01d95ff}
US	Urea ammonium nitrate (UAN)	agg	Sphera	Fertilisers	{8aad4bf6-4c56-4f94-9d13-c86fab06b0cb}
US	Triple superphosphate (TSP)	agg	Sphera	Fertilisers	{c684ff99-5662-4cd1-b28d-d6b3053c3cb6}
US	Calcium ammonium nitrate (CAN, solid)	agg	Sphera	Fertilisers	{0129673d-8cbd-49d3-990b-c90795e2a168}
US	NPK 15-15-15	agg	Sphera	Fertilisers	{6e463987-7963-4d6d-a5d3-0e50b93c592c}
IN	Ammonium nitrate (AN, solution)	agg	Sphera	Fertilisers	{7adee3a6-a1be-43c8-85b5-51aa40ded1d3}
US	Monoammonium phosphate (MAP)	agg	Sphera	Fertilisers	{d7e35f18-407f-45f2-843d-76d7852167c9}
US	Potassium chloride (agrarian)	agg	Sphera	Fertilisers	{8494b096-e9c1-4b12-959e-46d23d9da53f}
IN	Urea (agrarian)	agg	Sphera	Fertilisers	{b44b34b8-7949-4bab-bfb4-fb119b02d353}

US	Phosphoric acid (54% P_2O_5, agrarian)	agg	Sphera	Fertilisers	{f248cd05-a7f5-4954-97e0-b581355af9cb}
IN	Potassium chloride (agrarian)	agg	Sphera	Fertilisers	{0190da7c-f4d2-4da0-8399-c60ec26bf998}
GLO	Rock phosphate mix (32,4 % P_2O_5)	agg	Sphera	Fertilisers	{a9a40f47-b00c-48d9-9f96-ce44e6b7e6f7}
US	Limestone flour (50µm)	agg	Sphera	Minerals production	{3b6e72be-1eb3-4071-b968-b2c5b6c6121e}
IN	Limestone flour ($CaCO_3$; dried) (approximation)	agg	Sphera	Minerals production	{dbe5aa41-8282-48cf-947b-01bc1fa3d1d1}
RER	Limestone flour ($CaCO_3$; dried)	agg	Sphera	Minerals production	{28c77d66-cfac-454b-8a16-404dcc98eb67}
IN	Lime (CaO; quicklime lumpy)	agg	Sphera	Lime	{4534f45b-43eb-4295-b180-c660a38a87af}
US	Lime (CaO; quicklime lumpy)	agg	Sphera	Lime	{8807a563-ce17-4eeb-914f-567427c447c8}
RER	Lime (CaO; quicklime lumpy) (EN15804 A1-A3)	agg	Sphera	Lime	{1598e3ea-812d-4250-82ff-c477a7e57cfd}
US	Ammonia liquid (NH_3) with CO_2 recovery, by-product carbon dioxide (economic allocation)	agg	Sphera	Inorganic intermediate products	{c25e44cb-6c70-468e-bc76-0931fb8a9140}
RER	Potassium chloride (KCl/MOP, 60% K2O)	agg	Fertilizers Europe	Fertilizers Europe	{a2a8695e-968c-4341-922c-a007c8a8c56d}
RER	Diammonium phosphate (DAP, 18% N, 46% P_2O_5)	agg	Fertilizers Europe	Fertilizers Europe	{3e10ae2e-01f5-4e91-b098-8f9b4b44e119}
RER	Urea ammonium nitrate (UAN, 30% N)	agg	Fertilizers Europe	Fertilizers Europe	{c19713df-4bb3-4b84-ade8-49a244c24882}
RER	Ammonium phosphate (AP, 52% P_2O_5, 8.4% N)	agg	Fertilizers Europe	Fertilizers Europe	{d27713d1-a464-44f4-8585-1481870847d1}
RER	Raw phosphate (32% P_2O_5)	agg	Fertilizers Europe	Fertilizers Europe	{709cd7af-c2ee-4314-aea6-828fb9f295c5}
RER	Ammonia (NH_3)	agg	Fertilizers Europe	Fertilizers Europe	{f1c2e4cd-0d6c-40d2-a518-c0bf1ce39ce5}
RER	Ammonium nitrate (AN, 33.5% N)	agg	Fertilizers Europe	Fertilizers Europe	{c2c4ebba-358f-493e-83ba-71bffe847e9a}
RER	Urea (46% N)	agg	Fertilizers Europe	Fertilizers Europe	{a03a1819-f679-41e9-a6cb-c02ce874e6f8}

RER	NPK 15-15-15 (nitrophosphate route, 15N-15P205-15K20)	agg	Fertilizers Europe	Fertilizers Europe	{327e2d94-14c0-4610-9b19-dd776a6a85ad}
RER	Calcium ammonium nitrate (CAN, 27% N)	agg	Fertilizers Europe	Fertilizers Europe	{d069ee25-aebc-4cb5-a3b6-2b976e859d21}
RER	Triple superphosphate (TSP, 46% P_2O_5)	agg	Fertilizers Europe	Fertilizers Europe	{8d0007f0-9ad8-43b0-86e4-ebe6e9f9d0e6}
RER	Phosphoric acid (H_3PO_4, 54% P_2O_5)	agg	Fertilizers Europe	Fertilizers Europe	{fefe1855-2fb9-4bc0-874d-a72c3f54de71}
MY	Diesel mix at filling station	agg	Sphera	Filling station	{95f7992e-cca0-41fa-b510-06bc73969b0d}
DE	Diesel mix at filling station	agg	Sphera	Filling station	{f63987f3-9c75-49b5-9b94-99203725d66a}
CN	Diesel mix at filling station	agg	Sphera	Filling station	{97539829-e5d9-4278-b69b-de66133a94f2}
AU	Diesel mix at filling station	agg	Sphera	Filling station	{5fa4a1e0-3eba-4729-9e9e-4a98bdb294c6}
IN	Diesel mix at filling station	agg	Sphera	Filling station	{6c2c293e-ee47-4383-a385-c80f7f7d8bde}
FR	Diesel mix at filling station	agg	Sphera	Filling station	{5942368f-33e3-4859-8d1a-ba6bcd222c38}
RER	Diesel mix at filling station	agg	Sphera	Filling station	{99248ee9-3a59-47e4-b1f1-bb79067249ba}
NL	Diesel mix at filling station	agg	Sphera	Filling station	{2b730917-d41c-4b60-bd79-27f16df1f5a0}
RU	Diesel mix at filling station	agg	Sphera	Filling station	{7dd7f160-a88c-47b2-b7f4-ec271b8a0642}
BR	Diesel mix at filling station	agg	Sphera	Filling station	{ec3ec538-9f53-432a-bb54-54a7fb042dc4}
US	Diesel mix at filling station	agg	Sphera	Filling station	{a3ce3c6c-7b55-45e5-9f93-a202ad50622b}
GB	Diesel mix at filling station	agg	Sphera	Filling station	{3e2ba43e-2dac-4566-9a61-3e1b4553de00}
RER	Electricity grid mix	agg	Sphera	Electricity grid mix	{001b3cb7-b868-4061-8a91-3e6d7bcc90c6}
IN	Electricity grid mix	agg	Sphera	Electricity grid mix	{b9f24581-2fe8-4393-810c-4789a92b9c3b}
NZ	Electricity grid mix	agg	Sphera	Electricity grid mix	{16e91be2-1262-4026-9560-98d44198cba6}
AU	Electricity grid mix	agg	Sphera	Electricity grid mix	{907d77d0-4830-4e6d-b396-963c77b05470}
RU	Electricity grid mix	agg	Sphera	Electricity grid mix	{966be53a-4a87-4c97-bc17-b4d8416019bf}
NL	Electricity grid mix	agg	Sphera	Electricity grid mix	{ba65b4f5-b979-4609-81ff-d0e16d8d2e59}
RO	Electricity grid mix	agg	Sphera	Electricity grid mix	{e7ca53ec-792e-4573-92ca-9752658e8e9d}

AR	Electricity grid mix	agg	Sphera	Electricity grid mix	{592936e2-fb0e-4790-8571-bea763e5e475}
CN	Electricity grid mix	agg	Sphera	Electricity grid mix	{124e9246-9e84-4352-86b5-c08837e8cf92}
ES	Electricity grid mix	agg	Sphera	Electricity grid mix	{f0a6c237-873e-474e-a9cb-bcff8a6b3fe2}
ID	Electricity grid mix	agg	Sphera	Electricity grid mix	{f2081add-ee2d-4e73-9135-ffecebfc9991}
TH	Electricity grid mix	agg	Sphera	Electricity grid mix	{d51c571a-02e5-43a9-aa40-50833c329bc2}
VN	Electricity grid mix	agg	Sphera	Electricity grid mix	{56b47454-0b28-47ed-bf6a-09ca1593488f}
PL	Electricity grid mix	agg	Sphera	Electricity grid mix	{1598ea72-ae02-42fc-ae87-7dbe90df17ce}
PH	Electricity grid mix	agg	Sphera	Electricity grid mix	{fde7e82f-3ee1-49d9-9016-e93e91c942b7}
MY	Electricity grid mix	agg	Sphera	Electricity grid mix	{042eecc2-b098-4572-9a30-18e76cadc5de}
DE	Electricity grid mix	agg	Sphera	Electricity grid mix	{48ab6f40-203b-4895-8742-9bdbef55e494}
LK	Electricity grid mix	agg	Sphera	Electricity grid mix	{eb861ddf-c7f0-41bd-adea-d990d04e7078}
US	Electricity grid mix	agg	Sphera	Electricity grid mix	{6b6fc994-8476-44a3-81cc-9829f2dfe992}
CA	Electricity grid mix	agg	Sphera	Electricity grid mix	{69e79b16-bb66-41aa-8d2f-aacdfb84d42a}
BR	Electricity grid mix	agg	Sphera	Electricity grid mix	{ceb36eee-1612-4101-81a8-0fb8aeac9032}
BD	Electricity grid mix	agg	Sphera	Electricity grid mix	{242fceff-e74e-4821-a474-48f2171eb16c}
GB	Electricity grid mix	agg	Sphera	Electricity grid mix	{00043bd2-4563-4d73-8df8-b84b5d8902fc}
UA	Electricity grid mix	agg	Sphera	Electricity grid mix	{382ef030-ac09-4534-bbe5-452bc0b81493}
FR	Electricity grid mix	agg	Sphera	Electricity grid mix	{c8d7f695-1c5b-4f9a-8491-8c58c20c190f}
IT	Electricity grid mix	agg	Sphera	Electricity grid mix	{22b890c0-bd7b-47e4-b3a0-d4010c084cf5}
TR	Electricity grid mix	agg	Sphera	Electricity grid mix	{86c2ab55-7307-418c-bd11-b50166206ce9}
MX	Electricity grid mix	agg	Sphera	Electricity grid mix	{8c949961-24d2-42f6-ba8c-3511598a8ea3}
RER	Winter wheat cultivation (grain) (14% H2O content) - arithmetic average mix	agg	Sphera	Cereals (except rice), leguminous crops, oil seeds	{197fb3f2-d07f-4edd-b8ce-44f8cb2b2961}