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PestLCI Model: parameterization for scenarios of Brazilian agricultural production

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Jaguariúna, SP
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Foreword

Brazil has reached a prominent position in the international agricultural scenario in recent decades. It consolidated itself as one of the largest producers of commodities such as soy, maize, coffee, and sugar, among others. Scientific strengthening focused on agriculture and the development of suitable technologies for tropical countries, such as growing more than one crop per year in the same area, allowed Brazil to experience extraordinary growth driven by gains with increased yield. However, phytosanitary management is a major challenge faced by tropical agriculture. The dynamics of such a process under tropical conditions are intense, mainly due to the lack of severe winter, which enables the breaking of pest cycles.

Proper management of inputs applied to control pests, diseases, and weeds is a key factor to ensure agricultural production, both in quantity and quality. Thus, it is essential to understand pesticides' dynamics in the environment (soil, water, and atmosphere), as well as their potential impact on non-target organisms, since such a dynamic is influenced by the chemical features of different molecules, as well as by local soil and climate characteristics of areas where pesticides are used.

The present work describes the adaption and parameterization of the pesticide dispersion model in the environment 'PestLCI Consensus v.1.0'. The PestLCI model is a viable tool from an operational point of view, even for users without experience in the subject. At the same time, it reduces uncertainties related to the evaluation of the impact of pesticides on human health and the environment. This work will allow the expansion of environmental impact studies and provide subsidies for the development of safer technologies, allowing the creation of public policies and programs to rationalize the use of pesticides in food production.

This document contributes to the 2030 Agenda of the United Nations and meets the Sustainable Development Goal SDG 12, which aims to "Ensure sustainable production and consumption standards". More specifically, it meets goal 12.4, which seeks to "achieve environmental management of chemical products throughout their life cycle to minimize their negative impacts on human health and the environment".

Marcelo Boechat Morandi
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Summary

Introduction

Pesticides[1] are regulated and approved products used to control pests, such as insects and other arthropods, pathogens, and weeds which affect agricultural production. When applying pesticides, it is necessary to follow previously established recommendations listed on the label and package insert of these products. Additionally, these products must be used based on technical recommendations by qualified professionals, as to minimize risks to the environment and human health.

In order to assure safe usage, it is essential to understand the dynamics of pesticides in several environmental compartments (soil, water, and atmosphere), as well as their potential impact on non-target organisms. These dynamics are influenced by the chemical features of different molecules, as well as by the local soil and climate characteristics of the area where pesticides are used.

Several methodologies have been proposed to assess the impact of pesticides applied to agricultural crops. The 'PestLCI Consensus v.1.0' tool presented herein helps estimating pesticide ewwmissions in agricultural processes to prepare inventories for life cycle assessment (LCA) studies. This important environmental management tool was improved to enable the incorporation of the potential impacts of these compounds on agricultural production systems. In addition, the present work also aimed to parameterize relevant agricultural production scenarios for Brazil. With this, it is expected to lead to the improvement of LCA studies that address the possible impacts of pesticides on human health and the environment.

Life Cycle Assessment (LCA)

Life Cycle Assessment (LCA) is a method used to assess environmental impacts based on the amount of material and energy consumed by production processes and emitted to the environment throughout the life cycle of a given product. Life cycles comprise the extraction of natural resources, transformation and transport processes, up to product use and its final disposal stage. This impact assessment technique has strong scientific basis and is standardized by ISO 14040:2006 and ISO 14044:2006 (ISO, 2006a, 2006b).

LCA is divided into four stages: 1) Goal and Scope Definition; 2) Inventory Analysis; 3) Environmental Impact Assessment; and 4) Interpretation. The first phase defines the aim of the LCA study, its justification and target audience, as well as the intention to make comparisons and to publicize the study. The scope definition must ensure that study breadth, depth and detailing are compatible and sufficient to meet its aims. It includes the definition of the following elements: the product system[2] and its boundaries (Figure 1), function, functional unit[3], allocation procedures[4], environmental impact assessment method (LCIA), data requirement, assumptions and limitations (ISO, 2006a).

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1 LCA studies often use the term pesticide as synonym for agrochemicals. According to the Brazilian legislation, pesticides and the like comprise: a) products and agents associated with physical, chemical or biological processes, which are used in production sectors, in agricultural product storage and processing, in pastures, in the protection of forests (either native or implanted) and other ecosystems, as well as of urban, water and industrial environments, in order to change the composition of the local flora or fauna, as well as to protect them from the harmful action of noxious living beings; b) substances and products used as defoliants, desiccants, growth stimulators and inhibitors. Available at: http://www.planalto.gov.br/ccivil_03/leis/l7802.htm.

2 Product system: collection of unit processes with elementary and product flows, capable of fulfilling one or more defined functions, and of modelling the life cycle of a given product (ISO 14040, 2009).

3 Functional unit: quantified performance of a given product system to be used as reference unit (ISO, 2006a).

4 Allocation: fractionation of input or output flows of a given process or product system under investigation and one, or more, product systems (ISO, 2006b).

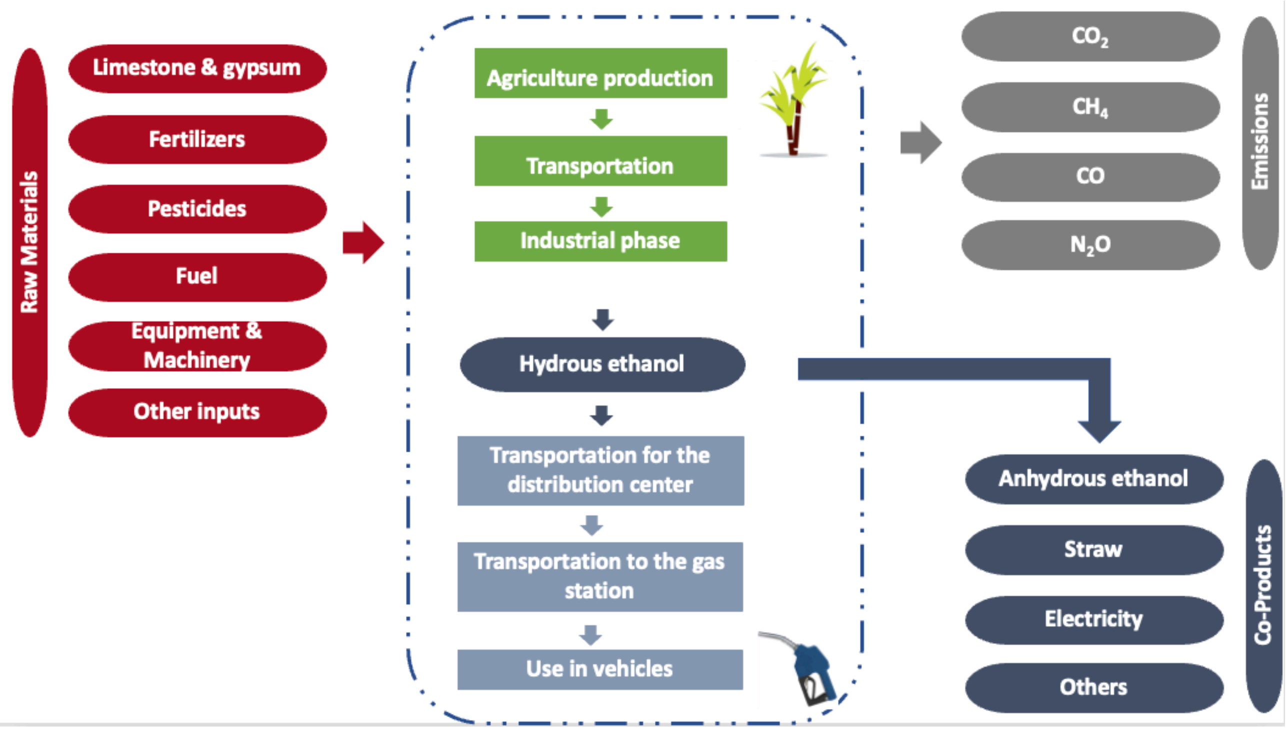

Figure 1. System boundaries: example developed for sugarcane ethanol (prepared by Mateus Chagas, Brazilian Biorenewables National Laboratory - LNBR, provided to the authors).

The inventory analysis stage comprises data collection and treatment to quantify input and output flows of material and energy that derive from processes taking place throughout a products' life cycle. The impact assessment stage focuses on evaluating the magnitude and significance of a products' potential environmental impacts. Finally, the interpretation stage focuses on evaluating the results, as well as on generating conclusions and recommendations (ISO, 2006b).

Life Cycle Inventories (LCI) correspond to sets of unit process[5] inventories linked by a reference flow[6]. A flowchart (Figure 2) is the first step to building process inventories and indicates material and energy input and output flows. Flow quantification results in the process inventory (Figure 3). Overall, input flows comprise primary (data collected straight from process managers) or secondary data (sector-related, statistical, or technical and scientific literature data), whereas output flows are estimated through models presenting different complexity levels.

[5] Unit process is the smallest element taken into consideration in Life Cycle Inventory analysis; input and output data are quantified for such an element (ISO, 2006a).
[6] Reference flow is the measurement of process outputs in a given product system; it is required to fulfill the function expressed by the functional unit (ISO, 2006b).

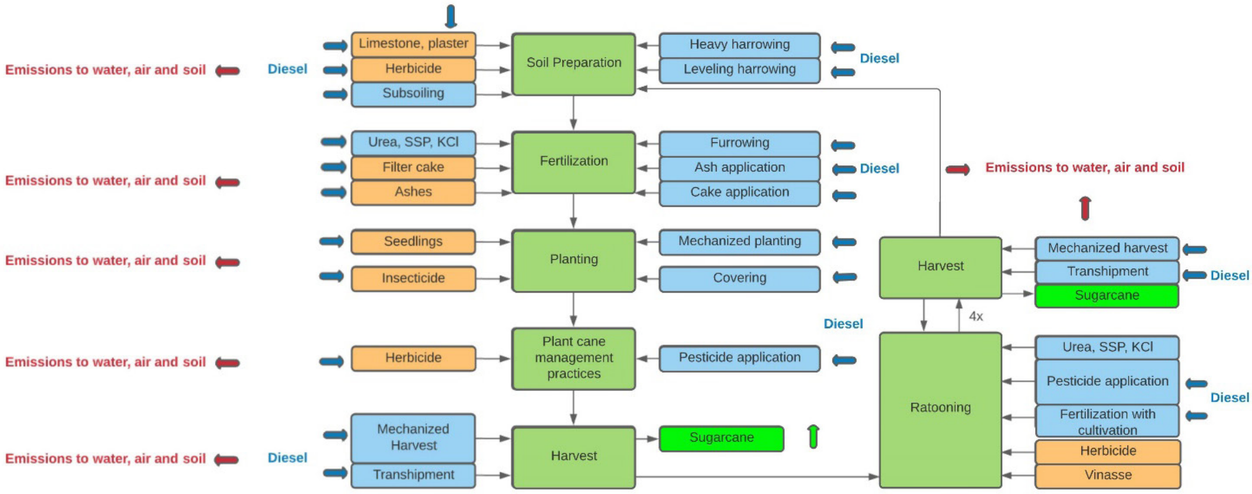

Figure 2. Process flowchart: example developed for sugarcane production (prepared by Juliana Picoli, Getúlio Vargas Foundation - FGV, provided to the authors).

The main international databases comprising life cycle inventories, such as Ecoinvent, (World Food Life Cycle Assessment Database (WFLDB), Agrifootprint and Agribalyse, often publish methodological guidelines to help estimate emissions from agricultural systems into the environment (Nemecek; Schnetzer, 2012; Nemecek et al., 2015; Van Paassen et al., 2019; Koch; Salou, 2020).

Ecoinvent 3.6 dataset documentation

sugarcane production - BR-SP

Exchange summary

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Reference products	Material for treatment	Byproduct classif.	Amount
sugarcane	no	allocatable product	1 kg
Inputs from technosphere			Amount
application of plant protection product, by field sprayer			1.75e-05 ha
ash, from combustion of bagasse from sugarcane			0.009 kg
fertilising, by rig fertiliser, sugarcane			9.98e-06 ha
fertilising, by stool splitter, sugarcane			3.09e-06 ha
field leveling, sugarcane			2.5e-06 ha
filter cake, from sugarcane juice filtration			0.0352 kg
furrow covering, sugarcane			8.91e-07 ha
furrowing, sugarcane			8.91e-07 ha
glyphosate			2.4e-06 kg
gypsum, mineral			0.00112 kg
harvesting, sugarcane			1.11e-05 ha
land use change, perennial crop			7.95e-06 ha
lime			0.00175 kg
limestone and gypsum application, by spreader			1.66e-06 ha
packaging, for fertilisers			0.011 kg
packaging, for pesticides			2.58e-05 kg
pesticide, unspecified			1.05e-05 kg
Inputs from technosphere			Amount
phosphate fertiliser, as P2O5			0.000356 kg
planting, sugarcane			1.61e-06 ha
potassium chloride, as K2O			0.0012 kg
sugarcane loading, by loader			1.39e-06 ha
sugarcane transfer, by dump cart			1.11e-05 ha
sugarcane vinasse application, by wheel reel irrigation			2.84e-06 ha
tap water			0.0112 kg
tillage, harrowing, by offset disk harrow			2.5e-06 ha
tillage, harrowing, by offset leveling disc harrow			2.5e-06 ha
tillage, subsoiling, by subsoiler plow			2.5e-06 ha
transport, tractor and trailer, agricultural			0.000241 ton*km
urea, as N			0.00107 kg
vinasse, from fermentation of sugarcane			0.529 kg
Inputs from environment			Amount
Carbon dioxide, in air			0.499 kg
Energy, gross calorific value, in biomass			4.95 MJ
Methane, non-fossil			5.67e-05 kg
NMVOC, non-methane volatile organic compounds, unspecified origin			0.000147 kg
Nitrogen oxides			6.51e-05 kg
Particulates, < 2.5 um			8.19e-05 kg
Particulates, > 2.5 um, and < 10um			0.000164 kg
Sulfur dioxide			8.4e-06 kg
Emissions to water			Amount
Cadmium, ion			7.77e-13 kg
Chromium, ion			9.64e-12 kg
Copper, ion			9.3e-12 kg
Lead			1.95e-11 kg
Nickel, ion			1.02e-11 kg
Nitrate			0.0027 kg
Phosphorus			3.8e-06 kg
Water			1.12e-05 m3
Zinc, ion			5.1e-11 kg
Emissions to soil			Amount
Cadmium			7.77e-09 kg
Chromium			9.63e-08 kg
Copper			9.3e-08 kg
Fipronil			4.99e-07 kg
Glyphosate			2.4e-06 kg
Lead			1.95e-07 kg
Nickel			1.02e-07 kg
Pesticides, unspecified			2.5e-06 kg
Emissions to soil			Amount
Sulfentrazone			7.49e-06 kg
Zinc			5.1e-07 kg

Figure 3. Process inventory: example developed for 1-kg sugarcane production. Source: Ecoinvent (2021).

Pesticide environmental fate

The environmental fate of pesticides applied on agricultural crops, as well as their partition into environmental compartments, encompasses complex and interrelated processes (Figure 4). However, several approaches have been employed in LCA studies, many of them extremely simplistic.

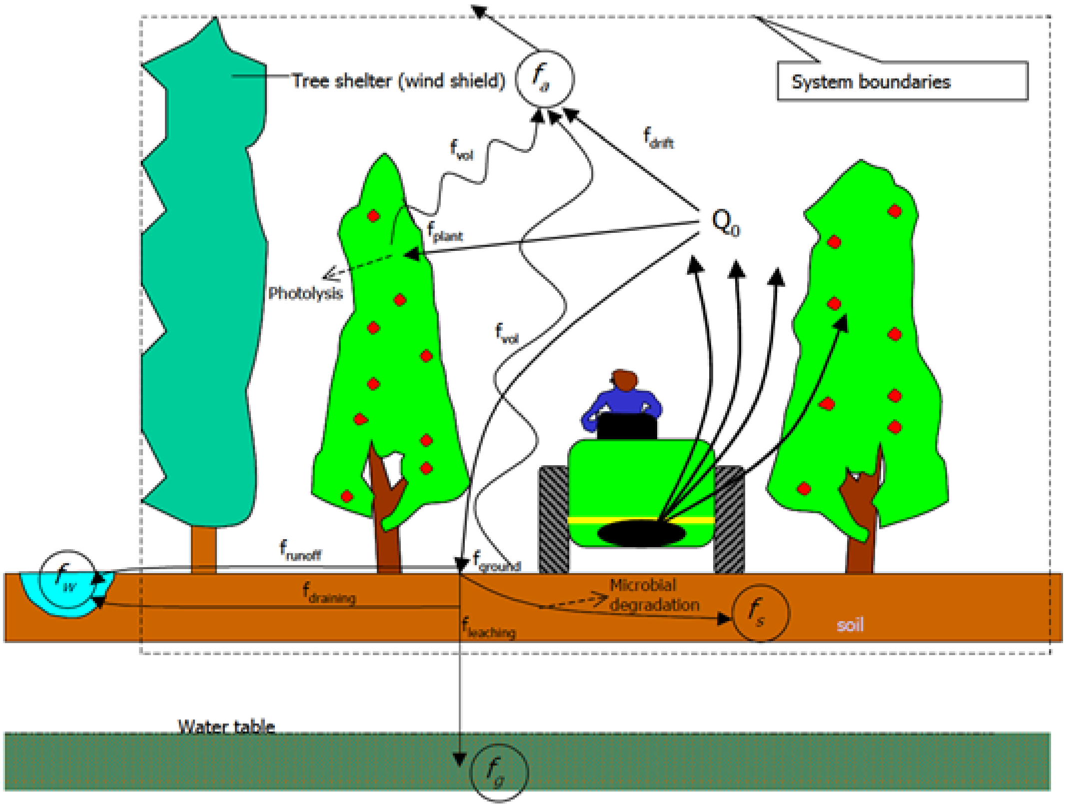

Figure 4. Dispersion routes after pesticide application.

Intermediate compartment fractions: *fdrift*: pesticide fraction lost due to drift; *fplant*: fraction reaching plants' surface; *fground*: fraction reaching ground surface; *fvol*: fraction lost due to volatilization; *frunoff*: fraction lost to surface water runoff; *fdraining*: fraction lost to surface water drainage; *fleaching*: fraction leached to groundwater. Final compartment fractions: *fa*: pesticide fraction reaching the air; *fw*: fraction reaching the surface of watercourses; *fg*: fraction reaching groundwater; *fs*: fraction remaining in the soil (Canals, 2003).

Different databases adopt different assumptions to partition pesticides into environmental compartments. Databases such as Ecoinvent, WFLDB (World Food Life Cycle Assessment Database) and Agribalyse take the allocation of total pesticide emissions to agricultural soils as premise. On the other hand, Agri-footprint suggests fixed pesticide fractioning for different environmental compartments: 90% for soil, 9% for air, and 1% for surface and underground water. However, the PestLCI model assigns a varying distribution of these pesticides into different environmental compartments, by taking into account chemical features of different molecules, application method, as well as soil and climate factors (Table 1).

Table 1. Comparison of pesticide partition model among different Life Cycle Assessment databases and models (Adapted from Fantke et al., 2019).

	Environmental Compartment	Approach (% emitted to the environmental compartments)									
		Ecoinvent	**Neto et al. 2013[1]**	**USLCI**	**USDA Ag-LCI**	**JALCA**	**WFLDB**	**Agribalyse MEANS**	**Agri-Footprint**	**PesLCI**	**PestLCI Consensus**
Agriculture soil	Agricultural soil	100	75	-	100	100	100	100	90	var.	var.
	Crop	-	-	-	-	-	-	-	-	var.	var.
Out of field	Air	-	-	~95	-	-	-	-	9	var.	var.
	Agricultural soil	-	-	-	-	-	-	-	-	-	var.
	Natural soil	-	-	-	-	-	-	-	-	-	var.
	Surface water	-	-	~5	-	-	-	-	1	var.	var.
	Underground water	-	-	-	-	-	-	-	-	var.	var.
	Others[9]	-	-	-	-	-	-	-	-	var.	var.

[1] Fixed emission fractions specifically estimated for viticulture.

The quality of results recorded for categories such as Ecotoxicity and Human Toxicity, at the Impact Assessment (LCIA) stage of LCA studies, depends on good resolution of pesticides' partitioning in different environmental compartments. Therefore, an adequate LCI model can lead to better results in these categories and enable more assertive decision-making processes.

PestLCI Consensus v.1.0 model

PestLCI Consensus v.1.0 is a modular model developed to estimate pesticide emissions from field application to different environmental compartments. The model calculates fractions of the applied pesticide emitted to air, soil, and to surface and groundwater, based on specific information about the application scenario, namely: application mode, culture and its developmental stage at application time, edaphoclimatic data about the treated area, as well as physicochemical properties of the applied pesticide (Birkved; Hauschild, 2006).

The model's modular structure enables the separate assessment of each process associated with the environmental dynamics of pesticides. Individual modules calculate pesticide input fractions and specific environmental destination processes, always considering the mass conservation principle. The modular structure has several advantages: (i) it allows modules to represent the state of the art for specific target processes and makes partial updates easier, as long as newly introduced modules respect the interface requirements of the remaining of the model; (ii) it enables the adaptation of the mathematical model to specific geographic conditions capable of influencing some destination processes; and (iii) it can also be used to calculate destination fractions to replace the relevant module of the model, in cases for which monitoring data are available for specific processes (Birkved; Hauschild, 2006).

Estimates of pesticide emissions to environmental compartments are based on two sets of distributions. Primary distribution takes into consideration the initial processes right after pesticide application (drift-related losses, deposition in leaves and soil).The secondary distribution based on the primary distribution results, and it integrates the processes taking place on the surface of crop leaves (degradation, volatilization, and absorption by plants) and soil (volatilization, degradation, leaching, and runoff). Then, the pesticide fractions emitted to the soil, air, surface and underground water, as well as to plant compartments, are estimated based on secondary distribution results (Dijkman et al., 2012).

Agricultural soil and surrounding areas can be considered part of the ecosphere (environment) or technosphere (production system) depending on the LCA study's goal and scope definition, and this can influence the final impact results. As an example, the adoption of agricultural soil as an ecosphere will change the emissions results of the pesticide under study, since the fraction estimated by the model in this environmental compartment will be accounted in the LCA impact assessment.

In comparison to other life cycle inventory approaches, the PestLCI Consensus v.1.0 model enables the integration of several specificities of the investigated scenario and reflects the state of the art for estimating pesticide emissions in LCA (Vazquez-Rowe et al., 2017). Thus, the model can point out variations in emission patterns caused by pesticide properties, edaphoclimatic conditions, and pest management strategies adopted by farmers. In addition, it can be used to assess the life cycle of agricultural product systems (Dijkman et al., 2012).

Selecting and Featuring Brazilian Production Scenarios to be Inserted in PestLCI Consensus V.1.0

Defining relevant agricultural crops to include Brazilian scenarios in the model

The relevance of the main crops that account for at least 70% of Brazilian agricultural production volume was used as criterion to select the Brazilian agricultural production scenarios included in the model. Municipal Agricultural Production (MAP) data of 2018 (IBGE, 2020a) were consulted to obtain this information; MAP values recorded for temporary and permanent crops were taken into consideration. In the first analysis, soybean, maize, cotton, and sugarcane were selected as temporary crops; accounting for 81.4% of temporary crop production values. Coffee, orange, banana, grape, and açaí were pre-selected among permanent crops, and they together accounted for 74.2% of production volume recorded for permanent crops.

The following crops were selected to be featured and included in the model based on the aforementioned criterion: sugarcane (accounting for 18.46% of production value), soybean (45.08%), maize (13.3%), cotton (4.52%), coffee (37.38%) and orange (15.51%). Besides the relevance of their production volumes, these crops were also selected based on the intensity of the demand for pesticide use in their production cycles.

Geographic mesoregions relevant to selected cultures

The current study has made the option for working with geographic mesoregions, which are territorial units with homogeneous physical, economic, and social characteristics (IBGE, 2020b). The mesoregions were selected based on their contribution to the national agricultural production values, recorded for the previously selected crops. Subsequently, all mesoregions identified in the crop-based analyses were summed; resulting in 35 mesoregions (Figure 5). After this definition, the main producing county in each mesoregion was selected (Table 2). This step was taken to facilitate identification of the representative soil in the corresponding county, which will be described in a further topic. The largest extension of planted area in 2018 was the adopted criterion, according to MAP data provided by IBGE (IBGE, 2020a).

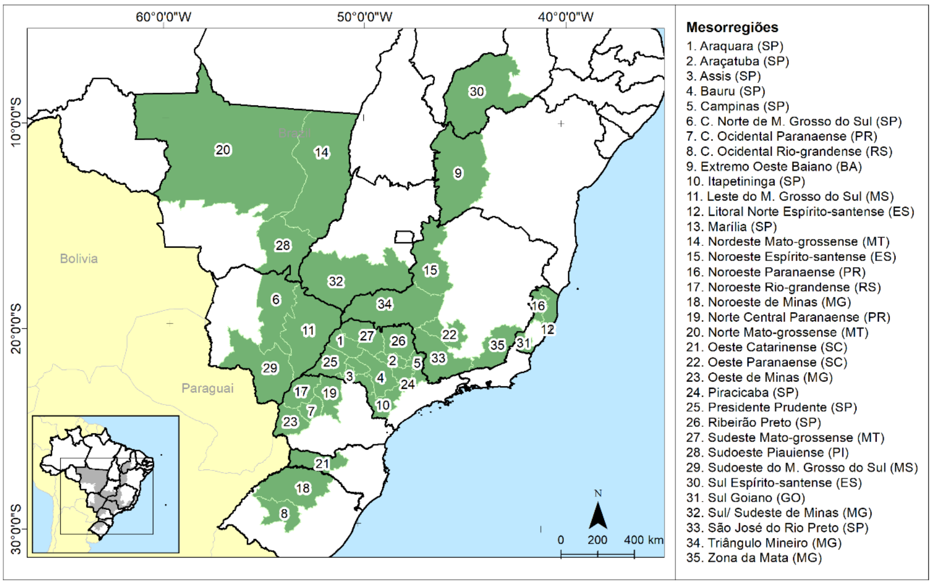

Figure 5. Geographic mesoregions (IBGE, 2020b) that, altogether, account for at least 70% of production values recorded for sugarcane, soybeans, maize, cotton, coffee, and oranges.

Table 2. Detailing geographic mesoregions (IBGE, 2020b) that, altogether, account for at least 70% of production values recorded for sugarcane, soy, maize, cotton, coffee, and orange.

UF	Mesoregion	Planted area in the mesoregion	IBGE Code	Main producing county	Planted area in the county	% of planted area in the county in comparison to the mesoregion
BA	Far West Bahia State (BA)	2,261,910.0	2928901	São Desidério	593,314.0	26.2%
ES	Northern Coast of Espírito Santo State (ES)	183,451.0	3203205	Linhares	46,385.0	25.3%
ES	Northwestern Espírito Santo State (ES)	128,187.0	3205176	Vila Valério	16,137.0	12.6%
ES	Southern Espírito Santo State (ES)	129,664.0	3203007	Iúna	15,894.0	12.3%
GO	Southern Goiás State (GO)	4,689,245.0	5211909	Jataí	537,500.0	11.5%
MG	Northwestern Minas Gerais State (MG)	909,475.0	3170404	Unaí	233,122.0	25.6%
MG	Triângulo Mineiro/Alto Paranaíba region (MG)	2,401,896.0	3170107	Uberaba	219,609.0	9.1%
MG	Western Minas Gerais State (MG)	213,807.0	3105103	Bambuí	30,268.0	14.2%
MG	Southern/Southwestern Minas Gerais State (MG)	858,363.0	3101607	Alfenas	36,683.0	4.3%
MG	Forest Zone (MG)	286,095.0	3139409	Manhuaçu	19,324.0	6.8%
MS	Center-North of Mato Grosso do Sul State (MS)	1,043,532.0	5007901	Sidrolândia	402,888.0	38.6%
MS	Eastern Mato Grosso do Sul State (MS)	684,811.0	5003256	Costa Rica	187,968.0	27.4%
MS	Southwestern Mato Grosso do Sul State (MS)	3,691,222.0	5005400	Maracaju	559,383.0	15.2%
MT	Northern Mato Grosso State (MT)	10,056,829.0	5107925	Sorriso	1,093,515.0	10.9%
MT	Northeastern Mato Grosso State (MT)	2,508,725.0	5107065	Querência	474,021.0	18.9%
MT	Southeastern Mato Grosso State (MT)	2,268,585.0	5107040	Primavera do Leste	444,199.0	19.6%
PI	Southwestern Piauí State (PI)	1,080,927.0	2201150	Baixa Grande do Ribeiro	247,687.0	22.9%
PR	Northwestern Paraná State (PR)	890,969.0	4100707	Alto Piquiri	57,602.0	6.5%
PR	Center-West Paraná State (PR)	1,129,878.0	4128005	Ubiratã	106,016.0	9.4%
PR	Center-North Paraná State (PR)	1,884,221.0	4113700	Londrina	106,135.0	5.6%
PR	Western Paraná State (PR)	1,993,459.0	4104808	Cascavel	198,563.0	10.0%
RS	Northwestern Rio Grande do Sul State (RS)	4,419,343.0	4313706	Palmeira das Missões	146,592.0	3.3%
RS	Center-West Rio Grande do Sul State (RS)	990,678.0	4322202	Tupanciretã	168,245.0	17.0%
SC	Western Santa Catarina State (SC)	643,890.0	4200101	Abelardo Luz	66,665.0	10.4%
SP	São José do Rio Preto (SP)	1,322,435.0	3500907	Altair	59,793.0	4.5%
SP	Ribeirão Preto (SP)	1,788,056.0	3531902	Morro Agudo	112,888.0	6.3%
SP	Araçatuba (SP)	683,489.0	3518206	Guararapes	52,019.0	7.6%
SP	Bauru (SP)	960,349.0	3521804	Itaí	62,643.0	6.5%
SP	Araraquara (SP)	483,215.0	3522703	Itápolis	53,606.0	11.1%
SP	Piracicaba (SP)	378,597.0	3538709	Piracicaba	54,081.0	14.3%
SP	Campinas (SP)	479,924.0	3510807	Casa Branca	60,972.0	12.7%
SP	Presidente Prudente (SP)	621,489.0	3542206	Rancharia	87,093.0	14.0%
SP	Marília (SP)	173,920.0	3540002	Pompéia	18,066.0	10.4%
SP	Assis (SP)	911,918.0	3546405	Santa Cruz do Rio Pardo	74,389.0	8.2%
SP	Itapetininga (SP)	450,264.0	3522406	Itapeva	166,205.0	36.9%

Survey on edaphoclimatic data about the selected mesoregions

Soils

MapBiomas Project data from 2018, collection 4.1, were used to define the soil type representative of each mesoregion (Souza Júnior et al., 2020). The aforementioned project focuses on classifying Landsat satellite images - pixel by pixel. This process helped generate annual information about land use and cover countrywide, on an annual basis, from 1984 to 2019 (Souza Júnior et al., 2020). The current study took into consideration classes such as “annual and perennial agriculture” and “semi-perennial agriculture” to generate agricultural maps. It is worth highlighting that 2018 was selected as the base year because it presented the most updated information available at the time the present study was still ongoing.

Information about soil types was extracted after the agricultural area of each mesoregion was defined, based on the intersection between the soil-type and agricultural-area information plan derived from both the MapBiomas project and the pedological map of IBGE’s Natural Resources Mapping (NRM) project, at scale of 1:250,000. It is worth emphasizing that, although pedological map presentation and image interpretation processes were carried out based on this scale, the thematic content matching the number of sampling points referred to a pedological survey conducted at a scale of 1:1,000,000 (IBGE, 2018). Figure 6 schematically shows the methodology used herein.

The soil survey conducted in agricultural production areas in each mesoregion was used to establish the most representative soil class in them. The soil parameters necessary to the survey were obtained from the Brazilian Soil Information System, a database coordinated by Embrapa, available at: https://www.sisolos.cnptia.embrapa.br/.

The list comprising the most representative counties (according to larger planted area) in these mesoregions was used to search the database. The search was conducted in descending order of planted areas until the representative soil profile was identified for each mesoregion. Once the soil profiles were identified, the following parameters required by PestLCI were obtained: density (average value of horizons up to one meter, kg m^{-3}), number of soil horizons to 1 meter depth; pH values, texture (% clay, silt and sand), and organic carbon content (%) for each horizon.

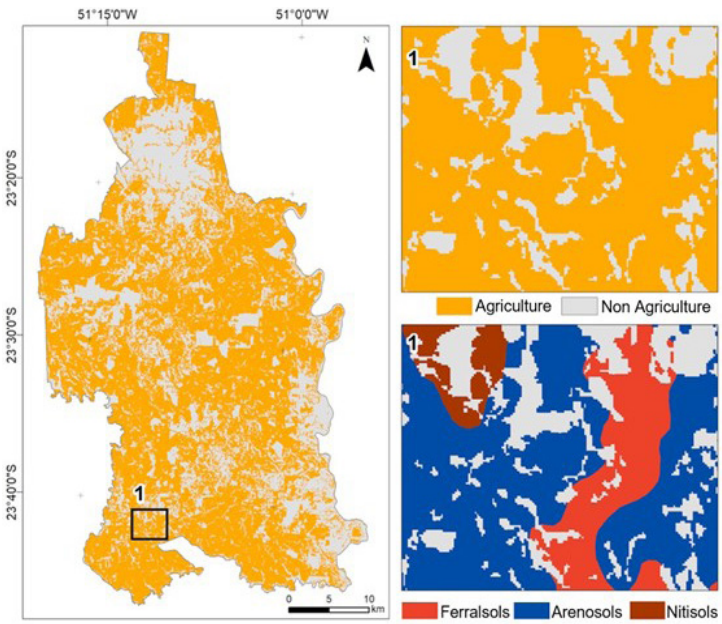

Figure 6. Outline of the methodology used to identify soil types in agricultural areas in Londrina County (PR), Center-North Paraná mesoregion. Subtitles in the order: orange: agriculture; grey: non agriculture; red: ferralsols; blue: arenosols; bown: nitosols

Climate

The following geographic and climatic parameters of the mesoregions covered in the current study were surveyed to meet the demand of the PestLCI Consensus v.1.0 model: latitude and longitude (in degrees E+, W-); altitude (m); mean temperature for each month of the year (°C); total annual rainfall (mm); mean rainfall on the rainy day of each month of the year (mm); mean annual rainfall on rainy days (mm); rainfall frequency (day^{-1}) of each month of the year; mean annual rainfall frequency; and potential annual land evaporation (mm $year^{-1}$). Tabulation comprised mean monthly values recorded for the investigated parameters, except for land evaporation values, which corresponded to the value accumulated throughout the year.

Three climatological databases were consulted for data compilation purposes. WorldClim was the first used database. It is a set of monthly climate data recorded from 1970 to 2000, interpolated at spatial resolution of approximately 1 km² (Fick; Hijmans, 2017); it is available at: https://www.worldclim.org/data/worldclim21.html). Subsequently, information about the mean number of rainy days (> 1mm) was extracted from the database compiled by Xavier et al. (2015). This set of monthly climate data, from 1980 to 2013, was interpolated at a spatial resolution of approximately 27.5 km².

Land evaporation values were extracted from the Global Land Evaporation Amsterdam Model – GLEAM climatological database (Martens et al., 2017), available at: https://www.gleam.eu/, which presents a model capable of estimating evapotranspiration compartments, such as land evaporation, separately. Land evaporation values used as input in the model corresponded to the mean value accumulated during the year. This monthly climate dataset, from 1980 to 2020, was also interpolated at spatial resolution of approximately 27.5 km².

All parameters were obtained in raster format and processed in GIS (geographic information systems) environment. Processing performed zonal-type operations, according to which the mean value, or the one accumulated in the year, recorded for the investigated parameters was tabulated in each mesoregion. Thus, mesoregions were featured in the climatological context of each month of the year, except for parameter "land evaporation". Monthly rainfall frequency was calculated by dividing the number of rainy days in the month by the number of days in the same month.

Survey on pesticides used in the selected crops

Representative pesticide molecules were established for the herein selected production scenarios based on market research information (provided by BASF S.A.) for pesticide application purposes. The criterion used to select the adopted pesticides comprised the potential area treated with these substances for each of the six selected crops. The choice made for this criterion, rather than for the amount of pesticide applied per area, was associated with the fact that the most modern molecules are overall applied at doses lower than those for older molecules, which would cause distortion in their relative application volumes. Therefore, pesticides accounting for 70% of the treated area in each investigated crop were determined. Filters were applied to exclude molecules repeated among cultures and those already found in the model's databases, since the PestLCI Consensus v.1.0 model database has a set of parameterized molecules. Twenty-seven (27) molecules representative of the production systems adopted in the main crops selected in Brazil were found in the current study and added to PestLCI databases (Table 3).

Table 3. Pesticide molecules added to the PestLCI Consensus v.1.0 model.

Molecule	Chemical Group	Use class
Abamectin	Avermectin	Insecticide/Acaricide
Acephate	Organophosphate	Insecticide/Acaricide
Acetamiprid	Neonicotinoid	Insecticide
Amicarbazone	Triazolinone	Herbicide
Benzovindiflupyr	Pyrazole carboxamide	Fungicide
Beta cyfluthrin	Pyrethroid	Insecticide
Bifenthrin	Pyrethroid	Insecticide
Carbendazim	Benzimidazole	Fungicide
Carbosulfan	Benzofuranyl methylcarbamate	Insecticide/Acaricide/Nematicide
Chlorantraniliprole	Anthraniamide	Insecticide
Diafenthiuron	Phenylthiourea	Insecticide/Acaricide
Difenoconazole	Triazole	Fungicide
Epoxiconazole	Triazole	Fungicide
Ethiprole	Phenylpyrazole	Insecticide
Fentin hydroxide	Organotin	Fungicide
Fludioxonil	Phenylpyrrole	Fungicide
Fluxapyroxad	Carboxamide	Fungicide
Isoxaflutole	Isoxazole	Herbicide
Metalaxyl-M	Acylalanine	Fungicide
Paraquat	Bipyridyl	Herbicide
Picoxystrobin	Strobilurin	Fungicide
Prothioconazole	Triazolinthione	Fungicide
Spinetoram	Spinosyns	Insecticide
Thiabendazole	Benzimidazole	Fungicide
Thiodicarb	Oxime methylcarbamate	Insecticide
Thiophanate methyl	Benzimidazole	Fungicide
Triflumuron	Benzoylurea	Insecticide

Data necessary to run the PestLCI Consensus v.1.0 model were organized for each molecule, namely: name, use class (insecticide, fungicide or herbicide), chemical abstracts service number (CAS), chemical category (acid, base or amphoteric substance), simplified molecular-input line-entry system formula (smiles), molecular mass (g/mol), solubility in water (g/l), vapor pressure (Pa), acid dissociation constant (pKa), octanol/water partition coefficient (log Kow), Freundlich coefficient standardized for organic carbon (Kfoc) or, sorption coefficient standardized for organic carbon (Koc), half-life dissipation in soil at 20°C (DT50)(days).

These data were extracted from the Pesticide Properties DataBase (PPDB[7], database developed by the Agriculture & Environmental Research Unit of University of Hertfordshire). Atmospheric OH rate parameters observed for molecules were extracted from the US National Library of Medicine. Kfoc value was assumed for molecules for which specific Koc value could not be found.

Once the culture, soil, climate, and pesticide databases were consolidated, as described above, the investigated scenarios were inserted in the PestLCI Consensus v.1.0 model. Hence, the model is ready to be used in pesticide partition into environmental compartments to build inventories for selected Brazilian crops and regions.

[7] Available at: https://sitem.herts.ac.uk/aeru/ppdb/en/index.htm

Using Brazilian Production Scenarios in PestLCI Consensus V.1.0

PestLCI Consensus v.1.0 model (Figure 7) can be accessed on the tool's online platform, available at https://pestlciweb.man.dtu.dk/; only in English. It is necessary to register as user, with e-mail and password, to log in to the system and access this tool.

Different tabs are available at the top of the model to enable navigating and using it. The initial (primary) distribution tab provides a generic and simplified way to calculate the distribution of emissions deriving from pesticide use into environmental compartments. Specific climate and soil data are not taken into consideration in this tab. The secondary emissions tab enables selecting soil and climate data for all specific regions found in the PestLCI platform, including the Brazilian ones. The 'secondary emissions' calculation option generates automatic results for the initial (primary) distribution.

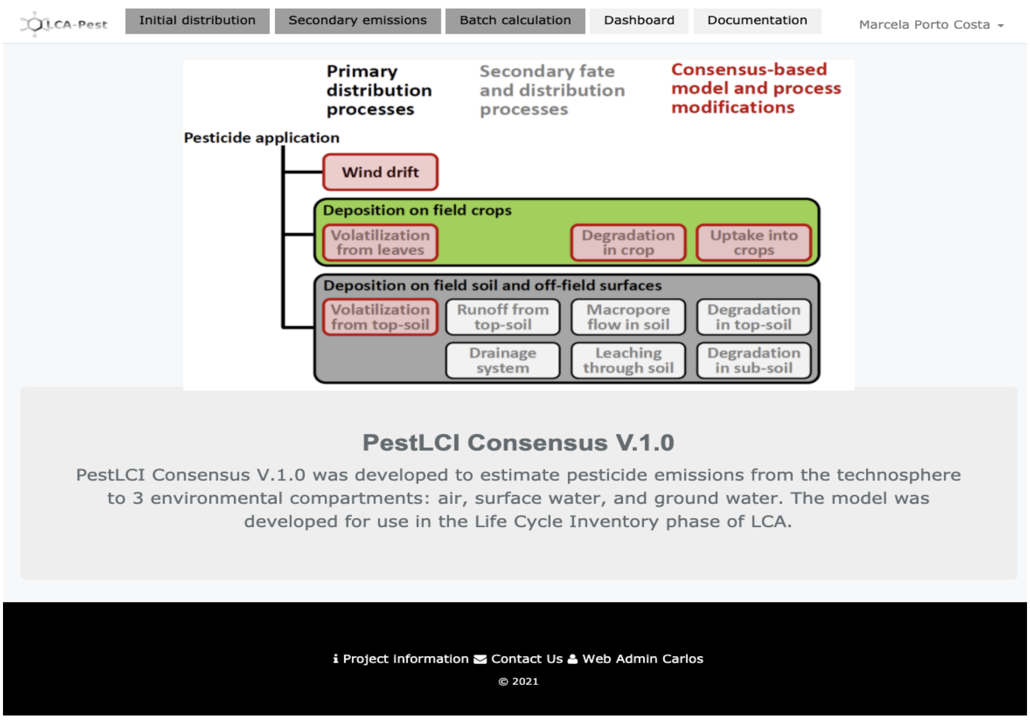

Figure 7. PestLCI Consensus v.1.0 input Interface.

The Dashboard tab provides an overview of all calculations generated by users in the tool. It also enables the review of all selected parameters, as well as exporting data from the generated simulations.

Simulating pesticide partition in environmental compartments, based on PestLCI Consensus v. 1.0

Initial (primary) distribution

Mandatory information, such as the name (title) of the calculation or project (e.g., 'Example 01: Soybean'), must be filled in to generate the initial (primary) distribution simulation (Figure 8). Such an identification is necessary to later retrieve the results in the dashboard. Subsequently, one must select the crop type (Crop type selection) - for example, soybeans belong to the "Oil-bearing crops" class, whereas coffee and sugarcane belong to the "Other permanent crops" class. Users must enter the fraction intercepted by leaf (Fraction intercepted by leaf) in the following field: this fraction derives from the selected crop developmental stage. By clicking on this field, users see a list with options, according to the selected crop and its developmental stage. The bare soil option should be used if the pesticide is to be applied at pre-emergence stage or right on the soil. The differentiation between cultivation systems (conventional, no-tillage, etc.) is carried out in a step described later in this document.

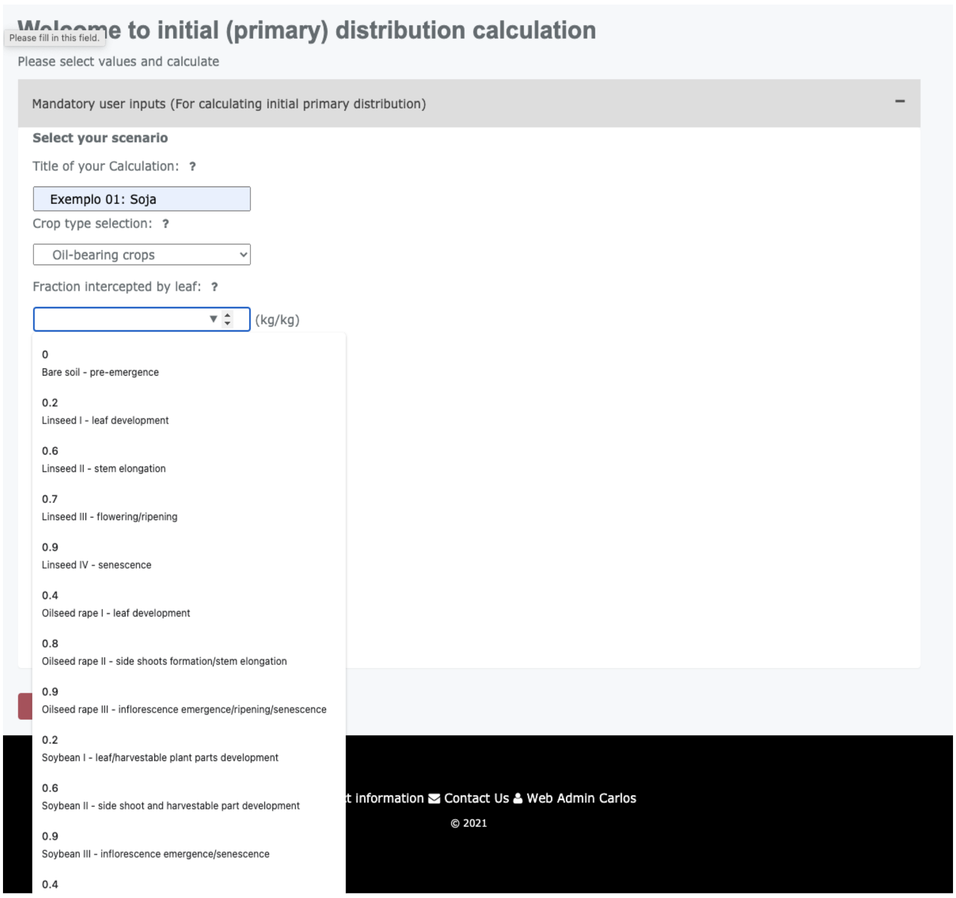

Figure 8. Initial (primary) distribution calculation. Required input parameters. Detail in fraction intercepted by leaves.

Subsequently, one must choose the pesticide application mode in the "Application methods" field (Figure 9). Once the application method is selected, a table is opened and it shows information about primary wind drift associated with that method, as well as about whether there is any drift reduction technique. If the method includes such a reduction, users must select 0% in the following field (wind drift reduction rate). Otherwise, users must select the most appropriate value for the investigated situation. Default values (standards) are suggested in this step.

The application dose must be reported in the mass of active ingredient applied in kg/ha. The system will assume the dose of 1 kg/ha if the application dose is not reported and results will depend on that dose. Users must enter details about the existence of buffer zone and the size of the area under analysis, in meters. Since Brazil has legislation focused on establishing permanent protection areas (PPA) of water courses, users can choose to use the PPA dimensions of the production system under investigation. This information is entered in the field (yes, ecosphere) when the PPA is outside the crop field. On the other hand, users must select (yes, technosphere) if there is a buffer zone inside the crop field and fill in the size of that zone in meters. After filling in these fields, users can generate primary emission results for the environmental compartments. Results are automatically saved to the Dashboard. With these results, users obtain output parameters that can be used in the impact assessment evaluation. However, the number of environmental compartments estimated in the initial distribution is smaller when compared to the results obtained by the secondary distribution.

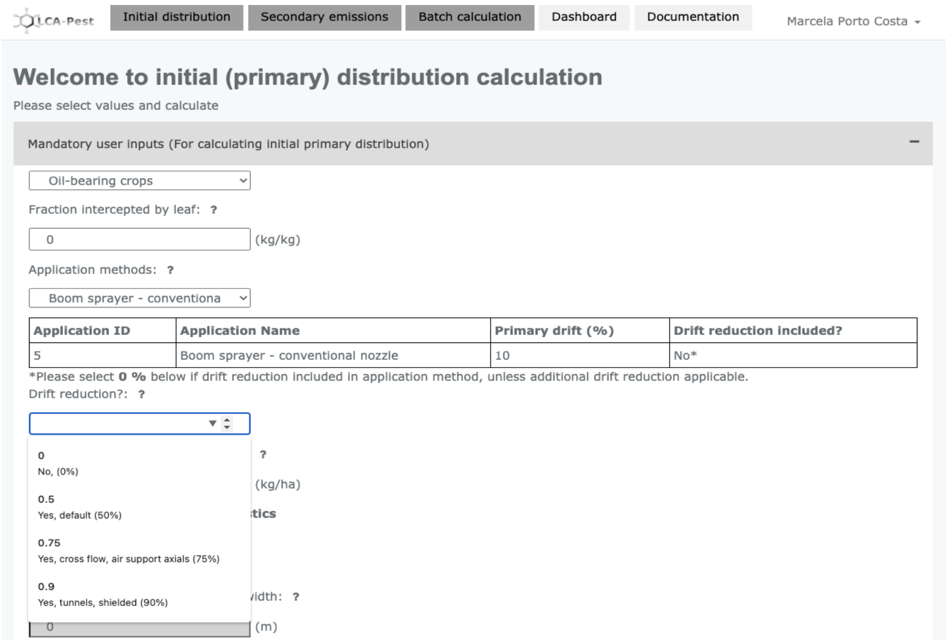

Figure 9. Initial (primary) distribution calculation. Required input parameters. Detail in application method and wind drift reduction rate.

Secondary emissions

The 'secondary emissions' tab has three sections. The first is composed of minimum data requirements to run the model, whereas the second and third sections provide other complementary input data and parameters that can be adapted based on default values established in the tool (Figure 10).

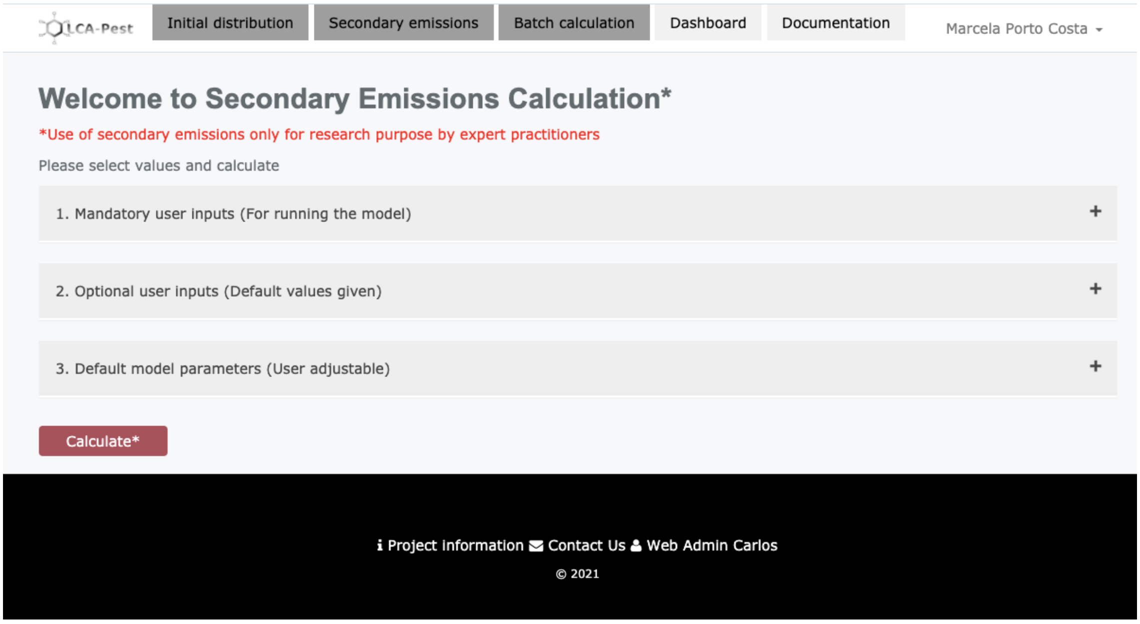

Figure 10. Filling in data in the secondary emissions calculation tab. It is mandatory filling in section 1, whereas it is optional filling in sections 2 and 3; if opted to use the standard values.

Section 1: Input data required to run the model

All fields in this section must be filled in for the model to run. Analogously to the primary simulation, it is necessary to define a title (title of your calculation), which will be used to retrieve the generated results. Figure 11 shows the calculation made for soybeans produced in Northern Mato Grosso State (Soja_Norte_MT).

The next mandatory field is the type of substance (pesticide) used. Insert the initial letters of the substance's name in the aforementioned field to find the desired substance on the platform, and a list of options will appear. These substances can also be searched based on CAS registration number. A table with the selected substance will appear and show its registration number, name, and classification (Figure 11).

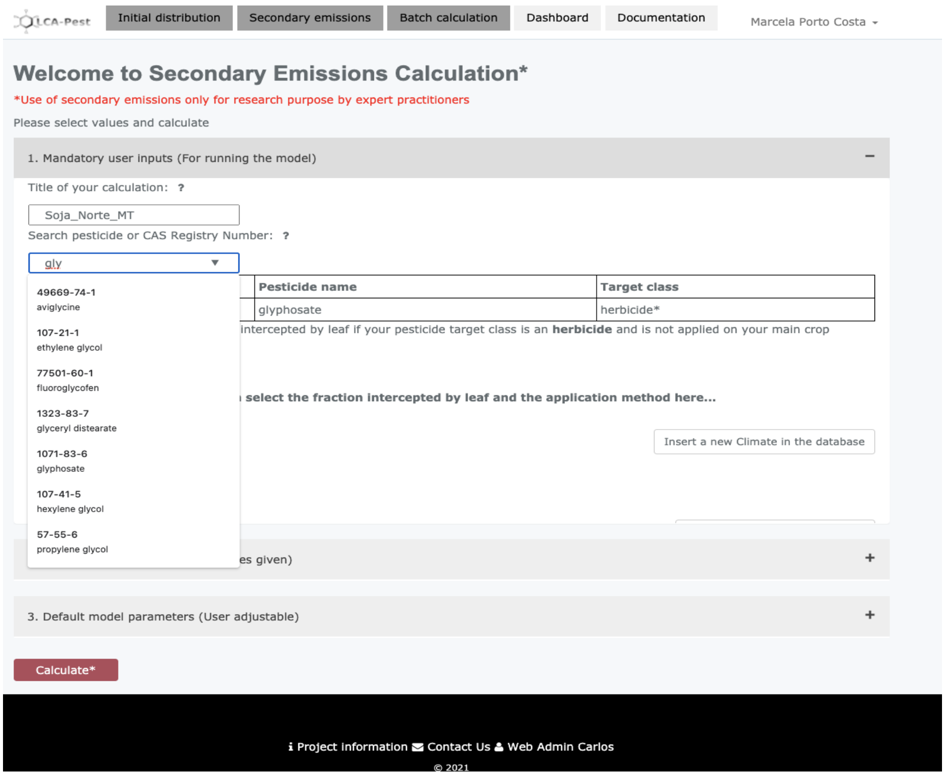

Figure 11. Section 1 of the secondary emissions calculation tab; mandatory filling. Study identification and search for pesticides for simulation purposes.

Crop class is the next field to be filled in, in the same way as described above. The ‘Fraction intercepted by leaf’ field will show several filling options, depending on the crop and on its developmental stage at the time of pesticide application. The ‘bare soil’ option must be selected if the product is applied on the soil prior to planting or at crop pre-emergence. The appropriate value must be selected, based on the crop developmental stage, if the product is applied on the crop. The application method and the wind drift rate must be filled in, in a similar way, as described above.

Subsequently, information on pesticide application time (month), as well as climate and soil data about the investigated region, must be provided. Climate and soil data from all 35 Brazilian mesoregions described above are available for selection. The nomenclature of Brazilian climates and soils is defined as: “USERDEFINED: Gov_Brazil_Name of region in English_climate/soil type in English” (Figure 12). Detailed soil and climate information about each mesoregion, as well as about the counties forming them, can be found at (https://cloud.sede.embrapa.br/owncloud/s/JNLqtGwt8zKESDy).

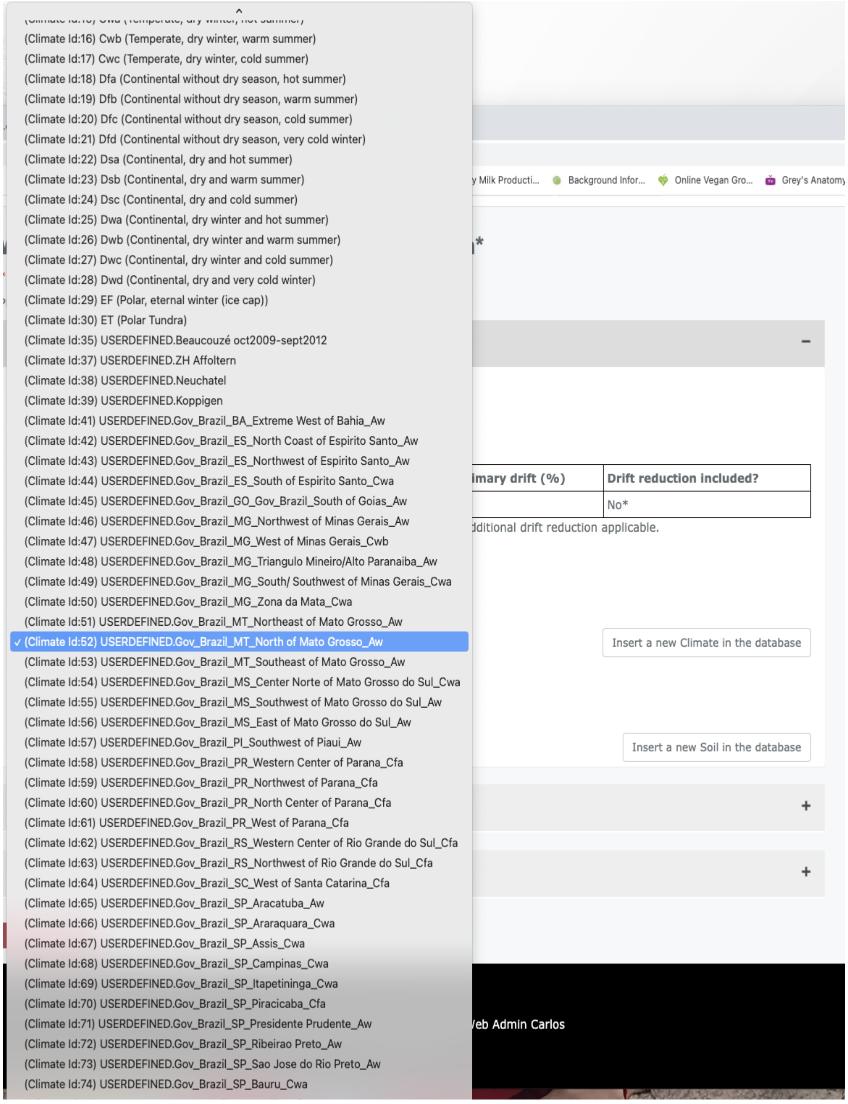

Figure 12. Nomenclature of 35 Brazilian mesoregions, together with soil and climate features, available in PestLCI Consensus v1.0.

Users can manually enter the specifications of the desired region by using the button on the right. However, in order to do so, it is necessary to enter all the requested information about climate and soil type. After climate and soil selection is carried out, Section 1 of the secondary emissions calculation tab is completed (Figure 13).

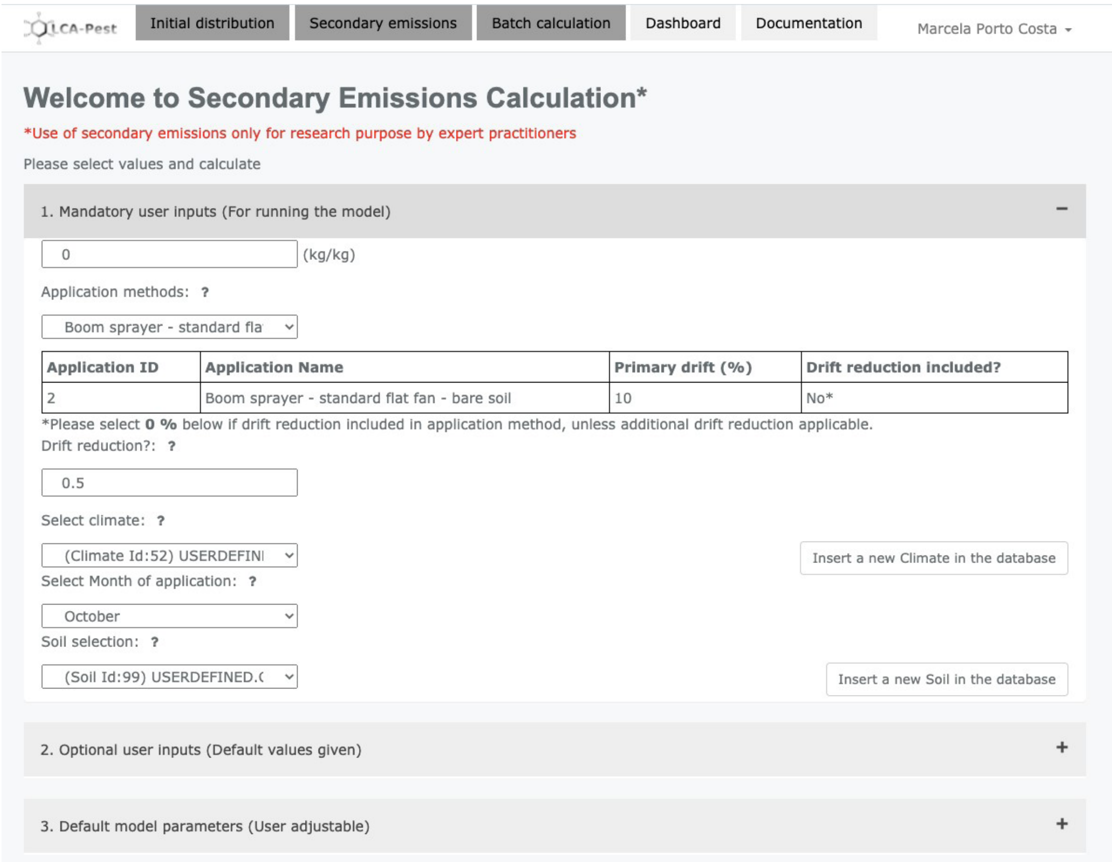

Figure 13. Section 1 completed. This section is mandatory to calculate secondary emissions in the model. Required input data comprise product-application month, as well as climate- and soil-type in the investigated region. Specific soil or weather data can be manually entered at this step.

Section 2: Optional Input Data

This section enables specifying input data based on the investigated area, as well as entering information about the buffer zone, as detailed for primary distribution calculation. This section also enables adapting the entry of data such as applied dose, treatment area size, as well as cultivation–area specifications such as slope and whether any soil preparation procedure was implemented (Figure 14). The parameters related to drainage (Depth of drainage and Drainage fraction), which have values established by the model, must be set to zero in scenarios where this practice was not used. In Brazil, different from European scenarios, this procedure is not common because of the usually high permeability of the soils.

Section 3: Adjustable Model Parameters (optional filling)

This section enables the adaptation of the model's calculation parameters based on the desired specificities. If these parameters are not modified, the system will use default values for the calculation process (Figure 15).

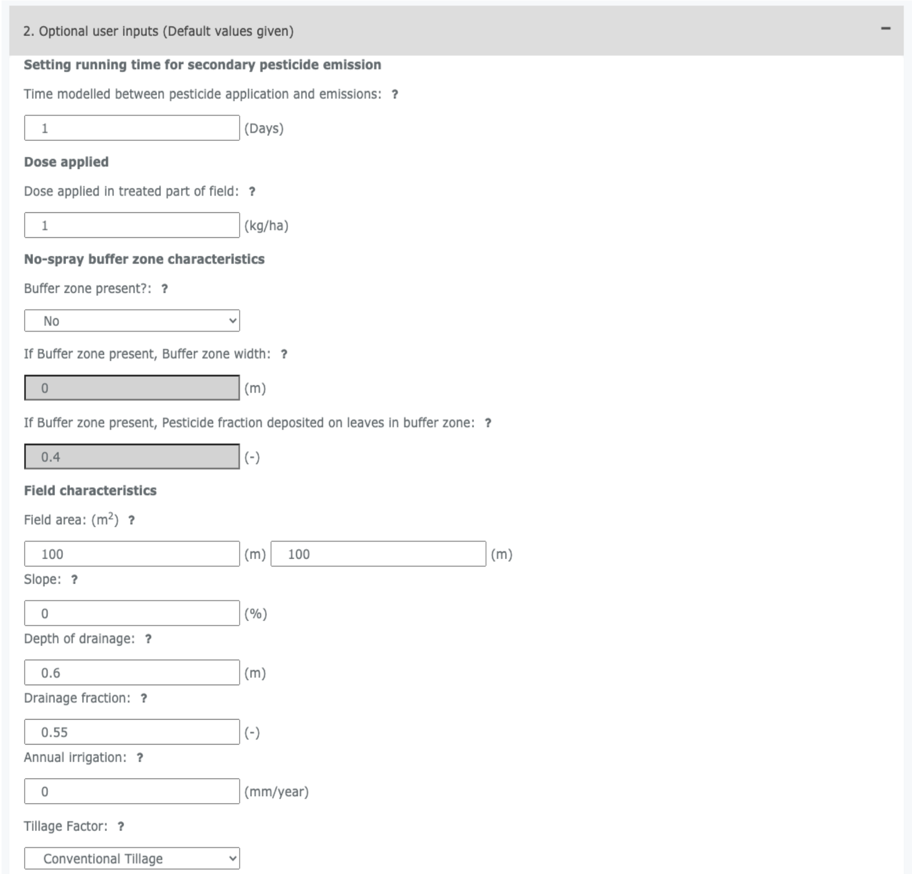

Figure 14. Section 2 of the 'secondary emissions' tab. Optional filling. If values are not adapted, the model takes into account default values.

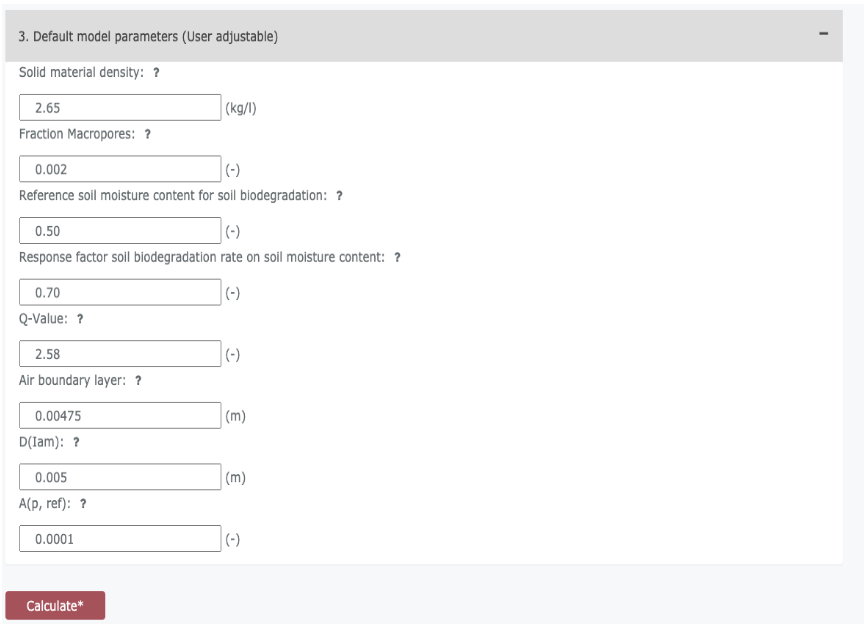

Figure 15. Section 3 of the 'secondary emissions' tab: Optional filling. If values are not modified, the model takes into account default values.

Results of initial (primary) distribution and secondary emission of pesticides in environmental compartments, based on PestLCI Consensus v.1.0

After the mandatory (Section 1) and optional (Sections 2 and 3) data filling processes are complete, calculations can be performed by clicking on the 'Calculate' icon. Results will be shown in tables, with emphasis on pesticide emissions for each environmental compartment.

Two tables of results will be available after secondary emissions' simulation and results' calculation; one table will show the initial distribution and the other one, the secondary emissions. Below the results, users can check the parameters selected for calculation purposes in 'Information about inputs selected' (Figure 16). At this stage, it is possible to change the secondary emission calculations or transfer the result to the dashboard. All calculations generated in this tool are automatically saved and remain available for viewing on the dashboard (Figure 17). If users delete one of the results, the information cannot be retrieved; thus, it is necessary to enter the data again.

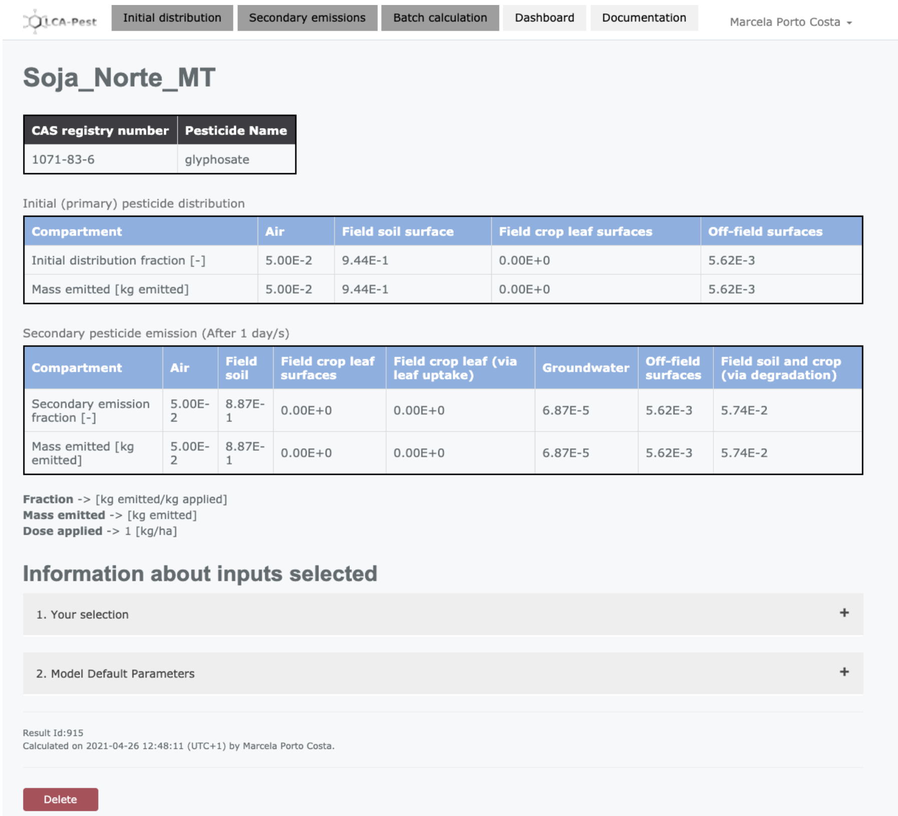

Figure 16. Results generated for initial distribution and secondary emissions.

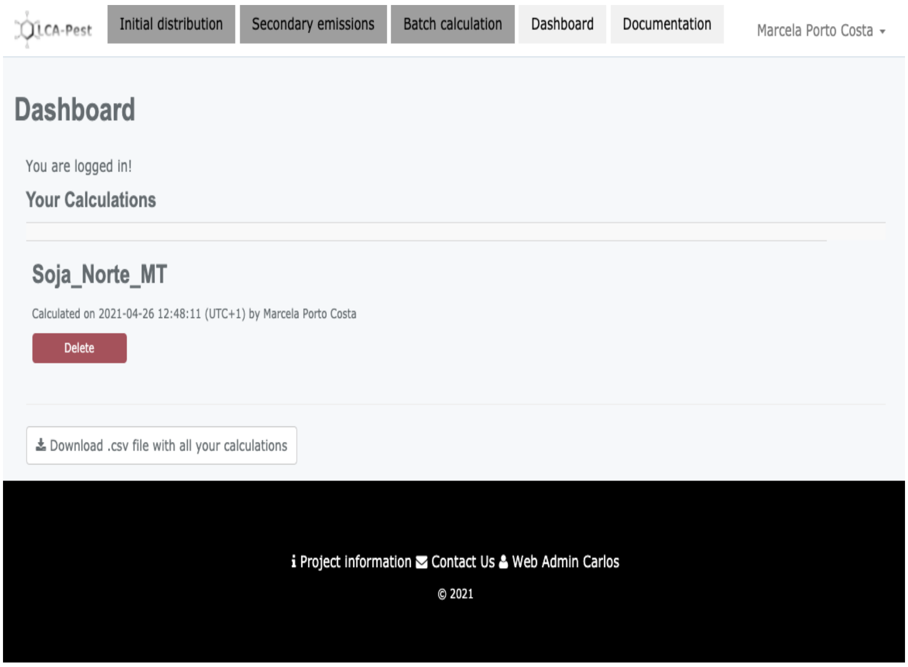

Figure 17. Dashboard holding all calculations generated by users.

Final considerations

The parameterization of tropical agricultural systems in PestLCI Consensus v.1.0 is a major advancement in environmental impact studies based on LCA. The current study took into consideration the main Brazilian agricultural production scenarios, which were physically featured and made available in the model database for LCA users.

The PestLCI model enables the reduction of uncertainties about the evaluation of pesticide impacts on human health and on the environment, and presents itself as viable operational tool to be even used by inexperienced users.

On the other hand, this tool enables LCA professionals to generate more qualified inventories and, consequently, more consistent results of potential environmental impacts, mainly in categories such as ecotoxicity and human toxicity.

The correct representation of pesticide dynamics in Brazilian tropical soils and climates will provide information quality gains, enable subsidies to help develop safer technologies, as well as public policies and programs focused on rationalizing the use of these compounds in order to improve food production sustainability and, consequently, to increase Brazilian agribusiness competitiveness.

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