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# A Commodity Supply Mix for More Regionalized Life Cycle Assessments

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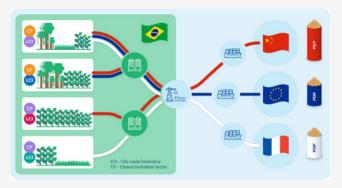
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ABSTRACT: Supply chain information is invaluable to further regionalize product life cycle assessments (LCAs), but detailed information linking production and consumption centers is not always available. We introduce the commodity supply mix (CSM) defined as the trade-volume-weighted average representing the combined geographic areas for the production of a commodity exported to a given market with the goal of (1) enhancing the relevance of inventory and impact regionalization and (2) allocating these impacts to specific markets. We apply the CSM to the Brazilian soybean supply chain mapped by Trase to obtain the mix of ecoregions and river basins linked to domestic consumption and exports to China, EU, France, and the rest of the world, before quantifying damage to biodiversity, and water



scarcity footprints. The EU had the lowest potential biodiversity damage but the largest water scarcity footprint following respective sourcing patterns in 12 ecoregions and 18 river basins. These results differed from the average impact scores obtained from Brazilian soybean production information alone. The CSM can be derived at different scales (subnationally, internationally) using existing supply chain information and constitutes an additional step toward greater regionalization in LCAs, particularly for impacts with greater spatial variability such as biodiversity and water scarcity.

KEYWORDS: life cycle inventory, spatialization, supply chains, biodiversity, water scarcity, soybean, Brazil, trade

#### ■ INTRODUCTION

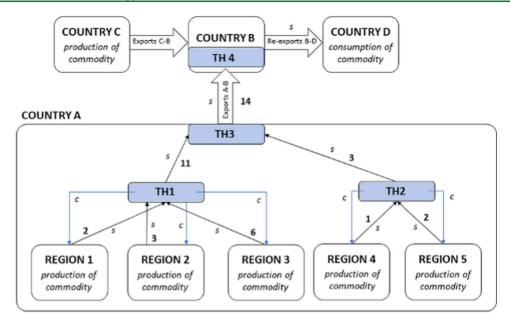
Life cycle assessment (LCA) is an approach that allows for the quantification of potential impacts of production and consumption processes throughout the life cycle of a product or service. LCAs follow a four-step process according to the ISO 14044 standard: (1) goal and scope definition, (2) life cycle inventory (LCI), (3) life cycle impact assessment (LCIA), and (4) normalization and interpretation. LCAs originally presented average potential impacts using generic site conditions, until the 1990s when the benefits of sitespecific approaches became an important topic of discussion. Since then, developments have highlighted the importance of representing site-specific conditions not only to account for differences in processes across multiple sites (e.g., electricity generation) but also because emissions (to soil, air, water) in different environmental settings and locations may lead to different impacts (e.g., terrestrial acidification, eutrophication).<sup>2,3</sup> The inclusion of site-specific information can, in turn, affect the conclusions of LCAs that would only be based on site-generic data.3

Regionalization in LCA refers to the efforts to move from site-generic to more site-specific information and involves (1) providing more regionally relevant information that is

applicable to both LCI (i.e., "inventory regionalization") and LCIA phases (i.e., "impact regionalization") and (2) accounting for spatial variability, particularly in elementary flows (or "inventory spatialization").<sup>3</sup> Ideally, site-specific elementary flows would match the spatial resolution of existing characterization factors, but practitioners can be limited by the availability of data or the resolution of impact assessment models while also facing trade-offs between selecting finer spatial resolution data and reducing uncertainty in the results. 4 Efforts to further regionalize LCAs have accelerated in recent years, with the inclusion of land and water use impact categories, leading up to the UN Environment's Life Cycle Initiative Global Guidance on Environmental Life Cycle Assessment Indicators (or Global Guidance, henceforth).5 Land occupation and transformation impacts require detailed information on biophysical conditions and spatial hetero-

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**Figure 1.** Supply chain of a commodity produced and exported from country A (exporter) to country B (importer) before being re-exported to country D. The commodity is sourced from several subregions within country A (regions 1–5) before supplying country B through the trade hub networks (TH1, TH2, TH3). Each region and country can both produce, supply (s), and consume (c) the commodity. Numbers in bold are those used in Table 1 to calculate the commodity supply mix.

geneity to quantify potential damage to biodiversity and ecosystem services. <sup>6,7</sup> Similarly, water consumption and degradation impacts are known to vary across river basins due to variability in human and ecosystem demand <sup>8,9</sup> or background chemical concentrations <sup>10</sup> affecting human health <sup>11</sup> or natural resources. <sup>12</sup> More systematic regionalization in LCAs has been accompanied by methods to reduce uncertainty from spatial variability in both elementary flows and characterization factors, <sup>13–17</sup> methods for prioritizing regionalization, <sup>18–20</sup> software solutions, <sup>3,21</sup> and standardization of spatial boundaries. <sup>22</sup>

Regionalization has been a key consideration for the increasing number of LCAs of food products. These LCAs require high-resolution information on regional practices, soil and water conditions for production, as well as environmental conditions for emissions to soil, air, and water to derive more regionalized impacts. Impact spatialization, for instance, through finer-resolution LCI, can lead to different impact scores, particularly in cases of spatially variable characterization factors. This finer regionalization can also reduce uncertainty in impact assessment results, which can be an important step for agricultural products. There example, Yang et al. show that a finer-scale LCI of corn production in the United States using county boundaries was beneficial in differentiating variability in water use impacts, while state boundaries were enough for greenhouse gas emissions.

Three important challenges remain, however, to allow for a widespread application of finer-resolution LCI to further regionalize LCAs: (1) many food products are made using ingredients derived from agricultural commodities, which are aggregated and shipped in bulk, thereby increasing the challenge in deriving a spatially explicit LCI from "farm-to-fork"; (2) products are delivered to consumers through complex supply chains that obscure the true source region(s) and therefore the information required to regionalize LCAs; (3) when performing an LCA of a more complex consumer product (milk replacements, packaged meat product, etc.),

practitioners may have limited information on the production process of the raw materials (e.g., soy or corn production), thus limiting the ability to estimate potential damage to biodiversity, ecosystem services, and water use, which are more regionally significant. To overcome the above challenges, much work to date has focused on mapping international supply chains using either physical trade models, <sup>32</sup> regionalized input—output models, <sup>33,34</sup> or data-driven subnational trade flow networks. <sup>26,35,36</sup> In many cases, a transformed commodity (e.g., livestock feed) is tracked in terms of its primary agricultural commodity (e.g., soy, corn) as a means to link producers with consumers in LCA. <sup>28,32</sup> These studies, however, do not typically include further industrialization of these final products and often miss consumer-facing life cycle phases (e.g., distribution, product use, and end-of-life).

Several options are available to practitioners to increase the regionalization of an LCA study, all of which implicitly attempt to detail the supply chain of the production system under consideration: (1) regional downscaling through field surveys or regional output percentages, (2) testing production and supply scenarios, or (3) supply mixes. Regional output percentages allow for spatialization of the LCI based on, for example, the production output to capture both inter- and intraregional movements of a commodity or product. 15 Production and supply scenario testing can provide insights into a set of production and supply conditions among different regions with distinct environmental settings (e.g., land, water use, climate) or supply chains. For example, Castanheira and Freire<sup>37</sup> tested land use change and transportation scenarios for Brazilian and Argentinean soybean exported to Europe. Consumption or supply mixes are now available in ecoinvent version 3 through market data sets,<sup>38</sup> where the LCI is available from the global supply and consumption of products. This last option is particularly convenient for practitioners with little or no information on where production activities occur; however, the data relies on global production and consumption

statistics and will miss important subnational spatial variability for commodity production processes.

In this paper, we introduce the commodity supply mix (CSM) derived from a systematic approach to improve regionalization in LCA using existing commodity supply chain mapping at the subnational level but applicable to other scales (subregional to international). Similar to existing approaches exemplified by electricity<sup>39</sup> and water mixes, <sup>40</sup> the CSM aims to generate regionalized LCI for LCA practitioners even in cases where information may be lacking on the production of a commodity that is used as an ingredient into a more complex product. First, we describe the concept of the CSM for improving regionalization in LCAs before applying the method using Trase<sup>36</sup> to a case study of land and water uses for Brazilian soybean consumed domestically and exported to China (Mainland), the EU, France, and the rest of the world (RoW). We expect the CSM to be a much needed option for practitioners seeking to improve regionalization in LCAs of complex agrifood products, particularly for the quantification of potential impacts to biodiversity and water use.5

## ■ METHODS

Commodity Supply Mix. Weidema et al.41 define a production mix as a combination of suppliers of a product to areas of production and define a supply mix as the additional link between this production mix and specific consumers. Following this definition, we describe the CSM as a tradevolume-weighted average representing the combined geographic areas for the production of a commodity (or source regions) that are destined to specific consumer markets for that commodity. The CSM relies on the mapping of commodity supply chains, either nationally or internationally, to determine (1) the spatially explicit location of potential source regions that are associated with elementary flows, (2) at a scale adaptable to regional characterization factors that (3) can be linked to consumers. The CSM relies on supply chain nodes where commodities are combined in bulk before being transported to the next node(s) (hereafter named "trade hubs"). The nodes could be whole countries when considering re-exports of commodities within the context of international trade but also grain storage facilities, processing plants, distribution centers, etc., when looking specifically at incountry processes. For instance, within a producing country A (Figure 1), a CSM can be derived subnationally considering source regions that act as both regions of production and consumption (regions 1-5) through trade hubs (TH1, TH2, TH3) within the country. A CSM can also be derived at the country level considering international trade partners. For example, country B (Figure 1) may import a commodity from both countries A and C before the commodity is re-exported to country D (interpreted as a "market"). In this international case, country C can be considered an international trade hub. The CSM therefore links production to a place of consumption (or market); it can be applied at any scale following the needs and availability of both elementary flow data and characterization factors defined in the LCA study's goal and scope, a coarse resolution being defined through country-to-country international trade, and the finest resolution being the multicountry subnational sourcing-to-country connections. The strength of the CSM for more regionalized LCAs is to match the region(s) (Figure 1) to a resolution that can match

existing characterization factors at a finer resolution than a country's borders.

In LCA, potential impacts are calculated following eq

$$I^{l} = \sum_{s,i} m_{i}^{s} CF_{i}^{sl} \tag{1}$$

where  $I^l$  is the potential impact for impact category l,  $m_i^s$  are the LCI elementary flows of emissions or resources extracted s in region i, and  $\operatorname{CF}_i^{sl}$  are the characterization factors for the impact category l identified by each elementary flow s for each region i. Current guidelines recommend that impact categories include potential damage to biodiversity and impacts to water scarcity, s for which the elementary flows are to be constructed from land and water uses (as s in eq 1) in ecoregions and river basins (as i). Using information on the commodity supply chain, the CSM distributes both elementary flows and characterization factors according to individual source regions linked to specific consumer markets j, as shown in eqs 2 and 3

$$I^{cl} = \sum_{s,i} CSM_i^{cj}(m_i^{cs}CF_i^{csl})$$
(2)

$$CSM_i^{cj} = \frac{S_i^{cj}}{\sum_{i}^{l} S_i^{cj}} \tag{3}$$

where  $CSM_i^{cj}$  (unitless) is the supply- or trade-volume-weighted share of source region i of commodity c for market j obtained by deriving the fraction of supply of the commodity among source regions  $S_i^{cj}$  that supply the commodity to market j. We apply eq 3 to a theoretical example (Table 1) to derive

Table 1. Theoretical Example of Calculation of the Commodity Supply Mix (CSM) of Country B Importing a Commodity from Country A Whose Supply Is Concentrated in Source Regions 1–5 (Figure 1)

regions	country A supply from sources	trade hubs	country A total supply to trade hubs	proportion traded to country B from trade hubs of country A	CSM: proportion traded to country B from country A regions
1	2	TH1	11	0.786	0.143
2	3				0.214
3	6				0.429
4	1	TH2	3	0.214	0.071
5	2				0.143

the CSM for a commodity from source regions in country A and exported to country B (Figure 1). The CSM is compatible with existing definitions of supply mix in ecoinvent<sup>38</sup> such that results may be integrated in ecoinvent's market data sets.

Case Study. We apply the CSM to a regionalized cradle-to-market attributional LCA of Brazilian soybean (as whole bean) focused on potential biodiversity damage from land occupation and impacts of water consumption from irrigation. The functional unit is 1 tonne of soybean produced in Brazil in 2017 that is destined to the main markets considering both the domestic market and Brazil's main international trading partners: China (Mainland), the EU (including the United Kingdom), France, and the RoW. The CSM is applied using the soybean supply chain map from the Transparency for Sustainable Economies (Trase) initiative<sup>36</sup> (see below) to

obtain the share of soybean supplied from different municipalities classified within Brazilian ecoregions and river basins. These supply chains are then combined with land and water use information to derive the elementary flows for each regionally specific characterization factor. Potential damage to biodiversity from land occupation was derived following eq 4<sup>7</sup>

$$I^{c,\text{occ}} = \sum_{i} \text{CSM}_{i}^{cj} (A_{i}^{c,\text{occ}} t^{c,\text{occ}} \text{CF}_{i}^{c,\text{occ}})$$
(4)

where  $I^{\varsigma,\text{occ}}$  (PDF yr tonne<sup>-1</sup>) is the potential damage to biodiversity from commodity c considering the LCI as the product of the area of land occupation in Brazilian ecoregion i,  $A^{\varsigma,\text{occ}}_i$  (m<sup>2</sup> tonne<sup>-1</sup>), and the occupation time ( $t^{\varsigma,\text{occ}}$  assumed to be 0.30–0.38 yr according to Flach et al.<sup>43</sup>) (see Table S1 in the Supporting Information for the full list of Brazilian ecoregions and Figure S1 for the map). Values of  $\text{CF}_i^{\varsigma,\text{occ}}$  (PDF m<sup>-2</sup>) are the ecoregion-specific characterization factors for land occupation from Chaudhary and Brooks<sup>44</sup> (cropintensive) (Table S1) based on the ecoregions from The Nature Conservancy.<sup>45</sup> Values of  $A^{\varsigma,\text{occ}}_i$  were derived from the 2017 inverse yield of each Brazilian municipality.<sup>46</sup>

Impacts of water consumption were expressed as a water scarcity footprint (WSF, m³ tonne<sup>-1</sup>) following Boulay et al.<sup>9</sup> using characterization factors specific to irrigation and following eq 5

$$WSF^{c} = \sum_{b} CSM_{b}^{cj}(WFI_{b}^{c}CF_{b}^{c})$$
(5)

where  ${\rm WFI}_b{}^c$  (m³ tonne<sup>-1</sup>) is the water footprint inventory of commodity c in each river basin b assuming a constant water consumption of 90 mm of irrigation per crop cycle (converted to m³ tonne<sup>-1</sup>) across the river basins following early planting practices in Brazil assumed to be widespread<sup>47</sup> for the purposes of the case study. Values of  ${\rm CF}_b{}^c$  are the AWARE characterization factors for irrigation, as defined in Boulay et al. (Table S2 and Figure S2).

We used Trase (trase.earth) for Brazilian soybean (v.2.5.0)<sup>48</sup> in 2017 to derive the CSM for the soybean supply chain and obtain the potential impacts of land occupation and water consumption from eqs 4 and 5. Trase is based on an improved supply chain map previously described by Godar et al., 49 which uses soybean exports and per-shipment trade data to link Brazilian municipalities of soybean production to import countries. In a first step, per-shipment trade records are used to identify the municipalities of taxation containing either farms, silos, or wholesale retailing (i.e., trader assets) by combining information from trade records (i.e., country of destination, cargo owner (trader), Brazilian state of production), tax records, and a list of trader assets. In a second step, the municipality of soybean production is identified by the minimum cost flow analysis using linear programming<sup>50</sup> that is optimized considering a combination of a trader's asset location (with silos identified using information on economic activity linked to the tax information), soybean demand (domestic and export demand), and transportation costs. The result is a Brazilian subnational supply chain map linking a municipality of production to a country of destination and the trader/port combination for each transaction. Municipalities acting as sources for our markets of interest in 2017 (Brazil, China, the EU, France, and the RoW) were then classified into source ecoregions and river basins following two classification methods (see the Uncertainty Analysis section) prior to

deriving the CSM for each market based on the supply volume of soybean exported.

Uncertainty Analysis. We accounted for three sources of uncertainty in the case study. First, we considered uncertainty in the classification of each municipality into ecoregions and river basins to ensure the results were not affected by zoning (also described as the "modifiable areal unit problem"). 14 The soybean supply chain mapped in Trase links a Brazilian municipality of production to the market of interest; as a result, a classification of each municipality within each ecoregion and river basin was necessary to select the appropriate characterization factors. However, a problem arises when attempting to classify a municipality located at the border of two adjacent ecoregions or river basins, leading to the selection of one characterization factor over another. We therefore considered two classification schemes following (1) the majority soybean area (labeled MS hereafter) and (2) the majority municipality area (MA). In the MS classification method, municipalities were part of an ecoregion or river basin if the majority of the soybean cropland area in the municipality (as determined using soybean crop maps from Song et al. 51 and available in Trase) were within that boundary. In the MA classification method, municipalities were part of an ecoregion or a river basin if the majority of the municipality's area was within their limits. Second, we accounted for uncertainty in  $t^{c,occ}$  from eq 4 (mean = 0.34 yr (125 days), upper bound = 0.38 yr (149 days), and lower bound = 0.30 yr (110 days)) following Flach et al.43 to represent the share of soybean occupation time in the annual crop cycle, as many regions of Brazil harvest more than one crop per year (soybean is often followed by corn). Finally, we accounted for the uncertainty in the characterization factors for land occupation (eq 4) as Chaudhary and Brooks<sup>44</sup> provide a distribution (mean, upper, and lower 95% confidence intervals) for each of their characterization factors. Impact assessment results assume no uncertainty in the inverse yield for land occupation  $(A_i^{c,occ})$  nor any uncertainty in the water consumption for irrigation (WFI<sub>b</sub> and CF<sub>b</sub>).

The Brazilian soybean supply chain map is based on trade data and a complete list of silos identified with company ownership that can be linked to exporters in the trade data. In addition, the links between the trade hubs and the municipalities of production represent those with the lowest cost of transportation, therefore illustrating the highest probable supply chain based on available information. In cases where these connections could not be made due to lack of information in the combined data sets (e.g., lack of information on the Brazilian state of production, missing trader, or ownership information), the soybean was labeled as having "unknown origin". In those cases, impacts were calculated using an LCI derived from the national mean yield. This means that the soybean of unknown origin was assigned the impact of the Brazilian soybean production mix.

Interpretation of Results. Impact assessment results are presented as a weighted average and as a probability density of impact scores from the spatial variability across ecoregions and river basins. The weighted average is obtained by taking the sum of the impact scores for each municipality supplying soybean to each market, weighted by their individual CSM. We interpreted these results as the impacts of the average tonne of soybean exported to each market. They are compared against the Brazilian soybean production mix or the weighted average obtained by summing the impact scores for all municipalities

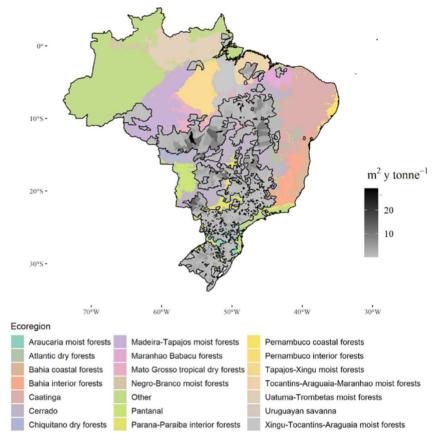


Figure 2. Spatially explicit life cycle inventory for land occupation (m² yr tonne<sup>-1</sup>) for Brazilian soybean exported to China in 2017. Values shown are specific to the majority soybean classification of municipalities into the ecoregions<sup>37</sup> and mean land occupation time.<sup>35</sup> Results for Brazil's domestic consumption and exports to the EU, France, and the RoW are shown in Figures S3–S6.

that produced soybean in 2017, 46 weighted by the contribution of each municipality to total production.

We also present the probability density of impact scores following the spatial variability of results for each municipality that produced and supplied markets with soybean, according to five cases. These cases are meant to represent different options following a gradual increase in information available on commodity sourcing:

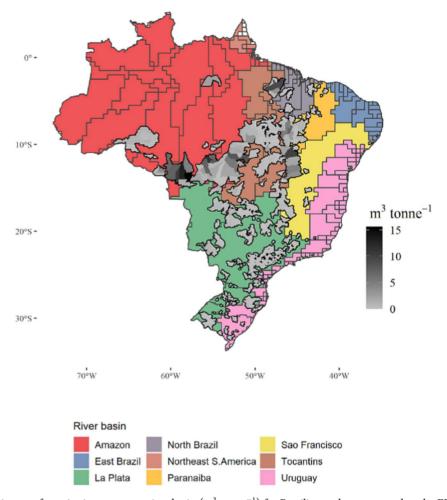
- "Production" case (P) for which impact scores are derived assuming an equal probability of soybean supply to markets. In mathematical terms, the values of the LCI (m<sub>i</sub><sup>s</sup> in eq 1) are obtained in each of the Brazilian municipalities and then divided by the number of municipalities (2275). This case can be interpreted as a typical option available for an analyst who would only have information on Brazilian soybean production.
- "Production mix" (PM) for which the probability of impact scores is distributed according to the contribution of each municipality to the total Brazilian soybean production. This case is similar to the P case, but for which a weighting factor accounts for the variability in soybean production across Brazil, assuming that markets have a greater probability of sourcing soybean from municipalities with greater production. This can also be interpreted as a typical option available for an analyst seeking to include more regional variability in the LCI.
- "Production mix to market" (PMM) is the same as the PM case but is qualitatively augmented by the information provided by the trade connections between

municipalities of soybean production and each market (i.e., trade volumes are not considered). In other words, the impact scores are obtained using information on municipal soybean production but reduced to those municipalities identified as suppliers of each of the markets. This case can be interpreted as an option resulting from in-country research or specific supply chain research carried out for the LCA.

- "Commodity supply mix" (CSM) for which the probability of impact scores follows the CSM.
- "Consumption boundary" (B) for which the probability of impact scores is derived assuming an equal probability of sourcing from the ecoregions or river basin boundaries identified in Trase. This case can be interpreted as an option resulting from general tendencies of supply focused specifically on ecoregion or river basin boundaries without additional knowledge on the amount of soybean sourced from these geographic boundaries.

In short, the above cases are meant to represent different options available for the LCA study considering limited information on regional production (as P, PM, B) or some information on supply chains (PMM, CSM).

Analysis was carried out, and graphs were generated using R statistical software  $(v.4.0.5)^{52}$  in R Studio (v.1.4.1103), with the *tidyverse*, and *patchwork* packages.



**Figure 3.** Spatially explicit water footprint inventory per river basin (m³ tonne<sup>-1</sup>) for Brazilian soybean exported to the EU in 2017. Values shown are specific to the majority soybean classification of municipalities into river basins. Results for Brazil's domestic consumption and exports to China, France, and the RoW are shown in Figures S7–S10.

Table 2. Commodity Supply Mix (CSM, Unitless) of Ecoregions and River Basins for Brazilian Soybean Destined to Each Market in 2017 (for Full Tables, See Tables S3 and S4 in the Supporting Information)<sup>a</sup>

	Brazil	China	EU	France	RoW
	MS-MA	MS-MA	MS-MA	MS-MA	MS-MA
Ecoregions					
Araucaria moist forests	0.178 - 0.179	0.131-0.132	0.023-0.023	0.097-0.110	0.087-0.086
Cerrado	0.489-0.482	0.414-0.404	0.490-0.482	0.485-0.477	0.474-0.466
Chiquitano dry forest	0.005-0.007	0.002-0.001	0.039-0.038	0.121-0.119	0.010-0.007
Parana-Paraiba interior forests	0.189-0.192	0.125-0.138	0.026-0.026	0.071-0.071	0.117-0.116
Mato Grosso tropical dry forests	0.048-0.049	0.061-0.069	0.239-0.249	0.097-0.110	0.132-0.144
Uruguayan savanna	0.074-0.070	0.121-0.113	0.001-0.001	0-0	0.053-0.052
other	0.017-0.019	0.145-0.144	0.182-0.181	0.227-0.223	0.128-0.128
River Basins (Number of Sub-basin	as)				
Amazon	0.109-0.113 (8)	0.156-0.158 (7-6)	0.552-0.560 (5-4)	0.705-0.706 (5-4)	0.313-0.315 (8-7)
La Plata	0.641-0.653 (3)	0.478-0.480 (3)	0.086-0.083 (3)	0.071-0.071 (2-1)	0.415-0.411 (3)
Sao Francisco	0.054-0.054 (1)	0.055-0.066 (1)	0.083-0.091 (1)	0.137-0.137 (1)	0.039-0.052 (1)
other	0.196-0.180 (15)	0.311-0.296 (20)	0.280-0.266 (16)	0.087-0.087 (3-2)	0.232-0.222 (18)
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<sup>&</sup>quot;Ranges represent the values obtained for the CSM following the majority soybean area (MS) and majority municipality area (MA) classification methods into ecoregions and river basins.

## **■** RESULTS

**Commodity Supply Mix and Life Cycle Inventory.** Brazil supplied 98.9 Mtonnes of soybean (as whole bean) in 2017, 93% of which was traced back to a municipality of origin (the remaining 7% could not be linked to a municipality of

origin). The CSM varied for each market: spanning 12 ecoregions and 17 river basins for domestically consumed soybean, 11 ecoregions (Figure 2) and 19 river basins for exports to China, 12 ecoregions and 18 river basins (Figure 3) for exports to the EU (including France), 7 ecoregions and 9

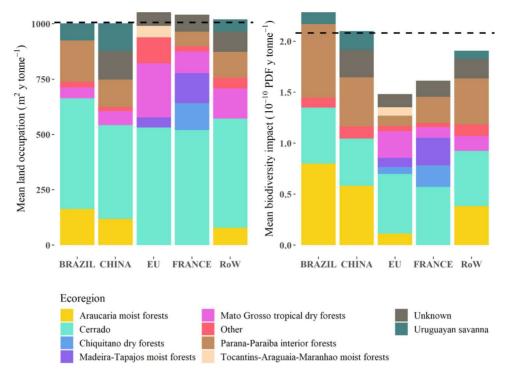


Figure 4. Life cycle inventory and potential damage to biodiversity for 1 tonne of soybean domestically consumed in Brazil and exported to China, the EU, France, and the rest of the world (RoW) in 2017. Results are broken down into the source ecoregions and compared to the Brazilian soybean production mix (dashed line) considering the mean characterization factors for Brazilian ecoregions.<sup>36</sup> and mean land occupation time.<sup>35</sup> Values shown are specific to the majority soybean area classification of municipalities into ecoregions.<sup>37</sup> Ecoregions hosting less than 4% of total life cycle inventory or damage to biodiversity were grouped into "Other". The ecoregion "Unknown" refers to trade data for which no known source ecoregion could be determined.

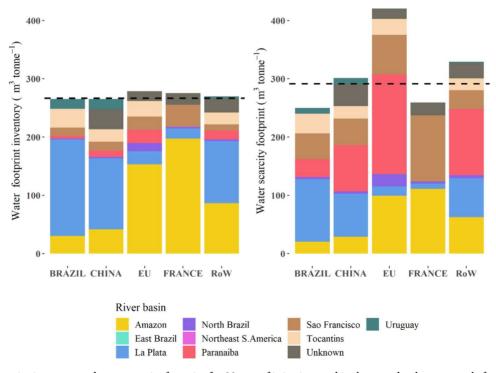


Figure 5. Water footprint inventory and water scarcity footprint for 90 mm of irrigation used in the crop development cycle for 1 tonne of soybean domestically consumed in Brazil and exported to China, the EU, France, and the rest of the world (RoW) in 2017. Results are broken down into source river basins and compared to the production mix (dashed line) considering the characterization factors for Brazilian river basins. Sub-basins were aggregated into larger basins for clarity (Table S2). The river basin Unknown refers to trade data for which no known source ecoregion could be determined.

river basins for France (Table 2), and 12 ecoregions and 20 river basins for exports to the RoW (values reported considering CSM ≥ 0.001; Tables S3 and S4 and Figures S3−S10). The Cerrado was the ecoregion that typically provided the majority of soybean to all markets with CSM values approaching 0.50. When combined with the Araucaria moist forests, Chiquitano dry forest, Parana-Paranaiba interior forests, Mato Grosso tropical dry forests, and the Uruguayan savanna, the sum of CSM values reached between 0.77 (France) and 0.98 (Brazil) (Tables 2 and S3). Similarly, the Amazon, São Francisco, and the La Plata were key source river basins for soybean, with combined CSM values ranging between 0.69 (China) and 0.91 (France) (Tables 2 and S4).

The land occupation LCI was 884–1120 m² yr tonne<sup>-1</sup> for Brazilian domestic consumption, 885–1120 m² yr tonne<sup>-1</sup> for soybean exported to China, 929–1176 m² yr tonne<sup>-1</sup> to the EU, 919–1041 m² yr tonne<sup>-1</sup> to France, and 900–1140 m² yr tonne<sup>-1</sup> to the RoW (Figure 4, left) (ranges represent the uncertainty from and land occupation times as per Flach et al.).<sup>43</sup> The water footprint inventory was 254 m³ tonne<sup>-1</sup> for Brazil (domestic market), 265 m³ tonne<sup>-1</sup> for exports to China, 279 m³ tonne<sup>-1</sup> to the EU, 276 m³ tonne<sup>-1</sup> to France, and 270 m³ tonne<sup>-1</sup> to RoW (Figure 5, left). These values can be compared to the results obtained for the Brazilian soybean production mix, which was 888–1125 m² yr tonne<sup>-1</sup> (for land occupation) and 266 m³ tonne<sup>-1</sup> (for water consumption) (Figures 4 and 5, left; production mix are represented by dashed lines).

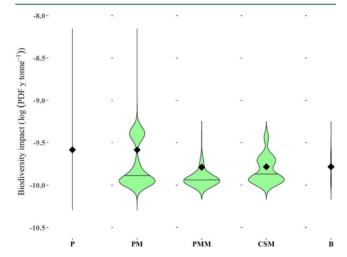
Life Cycle Impact Assessment. Spatially explicit land occupation LCI and water footprint inventory weighted by trade volume through the CSM were matched with the ecoregion and river basin characterization factors to derive the potential biodiversity damage from land occupation (Figure 4, right) and the water scarcity footprint (Figure 5, right) for each market. These results represent a weighted average potential biodiversity damage of land occupation or water scarcity footprint of soybean sourced from different Brazilian ecoregions and river basins and destined to the respective markets. The potential biodiversity damage of Brazil's soybean production mix due to land occupation was  $2.08 \times 10^{-10}$  PDF yr tonne<sup>-1</sup>, a value that was greater than the damage for soybean exported to the EU (1.48  $\times$  10<sup>-10</sup> PDF yr tonne<sup>-1</sup>), France  $(1.61 \times 10^{-10} \text{ PDF yr tonne}^{-1})$ , and the RoW  $(1.91 \times 10^{-10} \text{ PDF yr tonne}^{-1})$ 10<sup>-10</sup> PDF yr tonne<sup>-1</sup>) but lower when compared to Brazil's domestic market  $(2.28 \times 10^{-10} \text{ PDF yr tonne}^{-1})$  and exports to China (2.10  $\times~10^{-10}~PDF~yr~tonne^{-1})$  (all reported results consider both MS classification of municipalities into ecoregions, mean characterization factors, 44 and land occupation time)<sup>43</sup> (Figure 4, right, and Table S5).

Differences in impact scores were mostly due to less sourcing in the Araucaria moist forests and the Parana-Paraiba interior forests for both the EU and France, as well as a lower percentage of potential damage attributed to unknown sources in the soybean supply chain for the EU (5.6%) and France (7.3%) compared to that of China (12.9%) and the RoW (8.9%) and for which a national characterization factor was used. The water scarcity footprint of Brazil's soybean production mix was 292 m³ tonne<sup>-1</sup>. This value was greater than the scores obtained for soybean consumed in Brazil (250 m³ tonne<sup>-1</sup>) and soybean exported to France (259 m³ tonne<sup>-1</sup>) and the EU (421 m³ tonne<sup>-1</sup>) but lower than soybean exported to China (301 m³ tonne<sup>-1</sup>) and the RoW (329 m³ tonne<sup>-1</sup>) (range representing estimates from the MS

classification into river basins) (Figure 5, right, and Table S7). The water scarcity footprint was larger for soybean exported to the EU due to greater sourcing in the Paranaiba river basin in the southwest of the country.

Uncertainty and Probability Density. There was no statistically significant difference between impact scores when comparing distributions from the MS or MA classification of municipalities into ecoregions or river basins (t-test, p > 0.05 for all markets). When accounting for uncertainty in the characterization factors for biodiversity and the land occupation times in the LCI, the impact scores showed different ranges based on the market of interest (Tables S5 and S6). The EU's weighted average potential biodiversity damage was  $1.10-2.01 \times 10^{-10}$  PDF yr tonne<sup>-1</sup>, which was lower than any other market:  $1.73-3.03 \times 10^{-10}$  PDF yr tonne<sup>-1</sup> for soybean consumed in Brazil,  $1.20-2.18 \times 10^{-10}$  PDF yr tonne<sup>-1</sup> for the EU,  $1.43-2.56 \times 10^{-10}$  PDF yr tonne<sup>-1</sup> for the RoW, and  $1.58-2.80 \times 10^{-10}$  PDF yr tonne<sup>-1</sup> for China (values representing the range obtained with MS classification).

The probability of impacts from production (P) to boundary (B) cases showed differences in the ranges of impacts for each market (Figures S11–S19), but particularly for France where the probability of potential biodiversity damage and mean impact scores changed between PM, PMM, and CSM cases (Figure 6). Statistically significant differences in mean impact



**Figure 6.** Probability density of potential biodiversity damage (median (line) and mean (point)) for 1 tonne of soybean exported to France in 2017 following distributions obtained in five cases: production (P), production mix (PM), production mix to market (PMM), commodity supply mix (CSM), and boundary (B) as ecoregion. Values shown are specific to the majority soybean classification of municipalities into ecoregions<sup>37</sup> considering mean characterization factors<sup>36</sup> and land occupation time.<sup>35</sup> Probability densities for other markets and water scarcity footprints are available in the Supporting Information (Figures S11–S19).

scores were observed when comparing the production mix (PM) and the CSM cases for potential biodiversity damage (p < 0.05 for Brazil, China, and France) and water scarcity footprint (p < 0.05 for Brazil, EU, and France). The water scarcity footprint for soybean consumed domestically was the only market that had a significant difference in the mean impact score between the production mix for market (PMM) and CSM cases (Table S8).

#### DISCUSSION

## Improving Regionalization in Life Cycle Assessments.

The Global Guidance to include potential impacts to biodiversity and water use in LCA<sup>16</sup> implies a reliable level of regionalization that can differentiate spatial variability in ecoregion land occupation and river basin water use. Results from the CSM can facilitate the operationalization of the Global Guidance recommendations and improve LCI spatialization by applying the most regionally relevant characterization factors. Previous research has shown the importance of scale in representing the variability of LCI and its effects on impact assessment results for corn produced and traded within the United States. 26,28,29 While spatial variability may not be an important factor to consider for some impact categories (e.g., CO<sub>2</sub> emissions as in Yang<sup>29</sup>), other impact categories such as water scarcity<sup>28,29</sup> or biodiversity (this study) can benefit from further inventory spatialization. This spatial variability in the LCI is particularly relevant in the LCAs of more complex food products that rely on ingredients made from agricultural commodities such as soybean. The production and supply of these ingredients may be considered as a background process in the LCA of a food product for which information on spatial variability is often not available in online databases,<sup>29</sup> thus affecting the land and water use impact assessment results. Accurate information on exact sourcing of commodities can be challenging and costly to obtain. As a result, practitioners may need to make assumptions, consider different scenarios on the sourcing of ingredients, or may need to consult with experts to construct the supply chain of a specific product to include biodiversity and water use impacts (e.g., as in Milà i Canals et al.<sup>23</sup>). If widely applied, the CSM can help facilitate input data for LCAs using, for instance, the weighted average derived from the spatial variability to be included in the LCA of a product using Brazilian soybean as an ingredient.

The CSM relies on knowledge of the supply chain whose resolution (beyond country-country trade) can further improve LCI regionalization. It partially resembles what Yang<sup>15</sup> called the regional output percentage (ROP) approach in LCA for which a percentage output is allocated to different source regions. We see the use of a CSM to be adequate in cases where information is limited on the exact sourcing of a commodity, as is commonly the case for agricultural commodities. The CSM is applicable at the country level when considering international trade information, such as from COMTRADE (comtrade.un.org), from input-output, 33,34 or other physical trade methods, 32 but is more informative at a subnational sourcing level when information is available on source regions. In this study, we used Trase, which allowed for LCI regionalization considering the variability in soybean yields among the Brazilian municipalities, but other subnational supply chain maps may be used (e.g., as in Smith et al. 26 or Lin et al.<sup>35</sup>). Beyond applications for land occupation and water use, the CSM could also be complementary to identifying the source location of elementary flows for other impact categories. For instance, the results of this study could be complemented with production practices more generally (e.g., fertilizer application, management practices) to derive greenhouse gas emissions<sup>58</sup> or information relevant to social LCA as long as the information is available at the Brazilian municipality level.

Results obtained with the CSM show differences in biodiversity damage and water scarcity footprint among the

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different markets, while they also, in some cases, show differences with the results that would have been obtained using other assumptions about the soybean supply chain (e.g., production (P), production mix (PM), and consumption boundary (B)). The CSM could therefore be used as a method for prioritizing regionalization efforts in LCA such as that described by Patouillard et al.<sup>18</sup> using additional supply chain information in cases where spatial variability in the LCI is expected to have an important effect on the impact assessment results. For some markets, the impact scores were different when using a production mix compared to that of a CSM, highlighting the benefit to further spatialize the LCI while also allowing for a geographic hotspot analysis (see below). The uncertainty in the results of our case study came from the uncertainty in both the LCI and LCIA phases, considering differences in the occupation time (LCI) and the confidence interval of the characterization factors (LCIA). Uncertainty in the occupation time depends on either environmental factors, such as the photoperiod and accumulated rainfall, 59 or farming practices (e.g., double cropping), while uncertainty in the characterization factors depends on geographic variability within the same region. The lack of further information on farming practices (e.g., to resolve the occupation time per municipality) or the spatial variability in the characterization factors from Chaudhary and Brooks<sup>44</sup> shows a potential limit to further regionalization in our study based on existing information to resolve biodiversity damage across markets. Moreover, the results obtained from the CSM are only as good as the supply chain that is used to derive it. While Trase relies on detailed per-shipment trade data, the Brazilian soybean supply chain represents an average picture of relationships between municipalities of production and market in any given year with a certain level of stickiness, 60 keeping in mind that a small portion of these relationships could not be resolved due to missing information in the data.

Toward More Targeted Regional Hotspots. Different markets showed different sourcing patterns specific to their own soybean supply chain, which resulted in distinct compositions of the land occupation and water use elementary flows and impact assessment results. The results in this study for Brazilian soybean complement existing soybean LCAs with cradle-to-farm gate system boundaries by expanding boundaries to include markets. The regionalization of impacts also highlighted geographic hotspots to address potential biodiversity and water use impacts in geographic areas of concern. For instance, the Cerrado ecoregion was a source of soybean for all markets and is an important biodiversity hotspot, which has experienced rampant deforestation these past 20 years.<sup>65</sup> Similar to our case study, Green et al.<sup>66</sup> used Trase to assess the impacts of soybean exported from the Cerrado biome on endemic species as a means to highlight the role of importing countries on biodiversity. Here, we used Trase as an input into a CSM that considers all of Brazil's ecoregions and river basins to provide a more regionalized LCI and derive potential impacts from land and water uses following the methods recommended in the Global Guidance.<sup>5</sup> A geographic hotspot analysis in LCA can complement the current life cycle hotspot analysis, which has been the general objective of studies linking Brazilian soybean production to consumption centers, <sup>37,58,67</sup> and may be a bridge to combining both the territorial and supply chain perspectives in LCA. General efforts to improve transparency of supply chains can also underscore roles and responsibilities of countries and

companies as supply chain actors, as expressed in recent commitments to zero deforestation in supply chains.<sup>68</sup>

In this paper, we introduced the CSM as a method to facilitate further regionalization in LCAs while at the same time allowing for an allocation of impacts to markets. This proposed approach is relevant for analysts with limited visibility on production and export of commodities with complex supply chains seeking to apply recent guidelines on land and water uses in LCA. The case study of the Brazilian soybean production and export revealed a variability in potential impacts on biodiversity and water scarcity based on the main ecoregions and river basins, and the markets identified in the soybean supply chain. It also revealed how increasing information on the supply chain can help redistribute impact scores based on increasing information from the consumption perspective. Further examples of the CSM require greater understanding of national and international supply chains to provide a new set of LCI information for more regionally relevant LCAs using detailed and enhanced material flow analysis or input-output tables. Finally, the application of the CSM should also be tested in the context of consequential LCA and territorial LCA to assess its effect on decisionmaking.

#### ASSOCIATED CONTENT

## **Supporting Information**

The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/acs.est.1c03060.

Ecoregion and river basin maps of Brazil; spatially explicit life cycle inventory for ecoregion land use and water footprint inventory per river basin; probability density of potential damage to biodiversity and water scarcity footprint (PDF)

Comparison of impact scores from probability density curves (*t*-test) (XLSX)

Life cycle inventory results from the case study (XLSX)

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## **Author Contributions**

The initial draft of the manuscript was written by M.J.L. with input from all authors. Conceptualization was done by M.J.L., L.P., M.M., and C.W. Data organization and access were by B.A., P.L., and C.S. GIS work was done by P.L. and V.R. All authors have given approval to the final version of the manuscript.

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#### Notes

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#### ABBREVIATIONS

B consumption boundary case

CSM commodity supply mix (and case)

LCA life cycle assessment

LCI life cycle inventory

LCIA life cycle impact assessment

MA majority area classification

MS majority soybean classification

P production case

PM production mix case

PMM production mix to market case

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