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Spatial Variability and Uncertainty of Water Use Impacts from U.S. Feed and Milk Production

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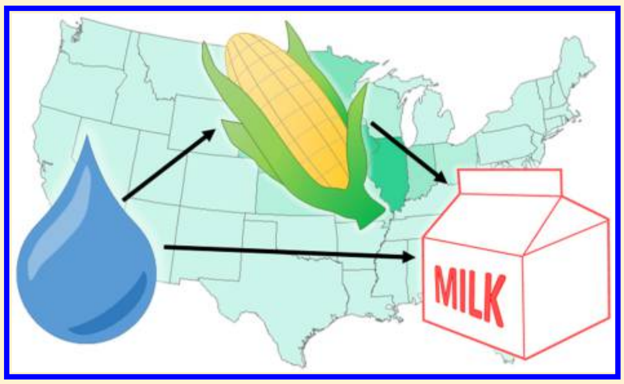
Supporting Information



ABSTRACT: This paper addresses water use impacts of agriculture, developing a spatially explicit approach tracing the location of water use and water scarcity related to feed production, transport, and livestock, tracking uncertainties and illustrating the approach with a case study on dairy production in the United States. This approach was developed as a step to bring spatially variable production and impacts into a process-based life cycle assessment (LCA) context. As water resources and demands are spatially variable, it is critical to take into account the location of activities to properly understand the impacts of water use, accounting for each of the main feeds for milk production. At the crop production level, the example of corn grain shows that 59% of water stress associated with corn grain production in the United States is located in Nebraska, a state with moderate water stress and moderate corn production (11%). At the level of milk production, four watersheds account for 78% of the national water stress impact, as these areas have high milk production and relatively high water stress; it is the production of local silage and hay crops that drives water consumption in these areas. By considering uncertainty in both inventory data and impact characterization factors, we demonstrate that spatial variability may be larger than uncertainty, and that not systematically accounting for the two can lead to artificially high uncertainty. Using a nonspatial approach in a spatially variable setting can result in a significant underestimation or overestimation of water impacts. The approach demonstrated here could be applied to other spatially variable processes.

INTRODUCTION

Water is essential for human development and for maintaining healthy ecosystems.[1] Yet the competition for scarce water resources is acute in many places, with human activity altering hydrologic systems.[2,3] Food production plays a significant role in this competition, as agriculture represents over half of fresh water withdrawals from rivers and groundwater,[4,5] Within agriculture, livestock have a significant share of the water use. Based on energy needs and time to maturity, the water requirements for livestock, on a mass basis, often exceed those of feed and human edible crops;[6] per calorie, nonbeef livestock products, including dairy, may have 50% more water demands than pulse crops.[7] The major part of this footprint stems from the animal feed production.[8,9] Hence, in the context of an increasing world population, assessing the water use impacts of feed and food production is crucial.

Life cycle assessment (LCA) and life cycle-based footprints aim to quantify environmental impacts of human activity.[10,11] For some environmental impacts, such as water use, it is crucial to take into account spatial differences.[12−14] Recent years have shown an increasing interest in spatializing both life cycle inventory, the compilation of exchanges and emissions to the environment, and life cycle impact assessment, the translation of the inventory to effects on humans, ecosystems, and resources.[15,16] Life cycle inventory databases such as ecoinvent are improving their regionalization features.[17] On the impact side, spatially explicit methods for impact analysis have been proposed[18−22] but are not commonly used. Pfister et al.[20] assessed water stress impact using characterization factors based on the ratio of fresh water withdrawals to availability, this ratio being computed on a regional scale, in order to account for the large spatial variability of water availability. Nitschelm et al.[23] suggested selecting an appropriate resolution for each impact

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category based on biophysical properties of the impact, but this is challenging for heterogeneous regions in the United States. Going one step further, Mutel et al.[16] presented a methodology for defining the optimal spatial scale and performing regionalized impact assessment.

One of the challenges with increasing spatial resolution in both life cycle inventory and life cycle impact assessment (LCIA) is to ensure a consistent interaction between these life cycle phases. Spatial scales of LCIA are often uniform grid cells, ecological regions, or hydrological units. The inventory often use political boundaries because of data availability. Inventory data can be disaggregated, but this leads to redundant unit processes and potential computational issues. Impact factors may be aggregated to match inventory resolution, but these aggregated values may miss important spatial differences.[15] In addition, uncertainty analysis of life cycle inventory data is relatively common (e.g., ref 24), but it is rare for impact analysis.

There has also been growing interest in tracking the relationship of economic activities and the location of their impacts.[25,26] Multiregional input-output approaches have been used in LCA contexts for water (and other) impacts of Dutch dairy production[27] and Swiss food consumption.[28] These analyses use trade data at a national level, using characterization factors aggregated from more highly resolved impact models. National average characterization factors for water stress may, however, not be appropriate for large countries such as U.S. with spatially variable water resources.

While there has been extensive work on virtual water transfers related to agricultural products (e.g., refs 29−31), these approaches do not easily allow impacts or inventory to be disaggregated throughout the supply chain. In this paper, we use water stress as an example of a spatially variable impact factor, in parallel to ongoing characterization efforts to improve the link between water use and impacts on human health and ecosystems.[10,32] Furthermore, we focus on *consumptive* water use; in the parlance of the Water Footprint Network, this is blue water.[31] Green water, precipitated water that may be evapotranspirated by plants, wild or cropped, is typically not considered in LCA, and gray water, a theoretical water to dilute contaminants to acceptable levels is captured in LCA via other impact categories.[20,27,33,34]

Crop production in the United States presents a unique spatial challenge to determine inventory, impact or water footprint, since irrigation requirements for feeds can vary by orders of magnitude across the U.S. Livestock, and specifically dairy, products are even more complicated, with feed composition and provenance varying geographically as well. The nation comprises heterogeneous territories with diverse climates, cropping practices, feeding practices, etc., which are not captured in existing input−output databases. Therefore, this analysis requires a spatially explicit approach to model feed production, trade, consumption, environmental impact, and uncertainty of water deprivation. Assessing the water use impact of feed for the U.S. national milk production is therefore a useful case study to illustrate the spatial analysis of water scarcity impacts.

This work aims to develop a framework for spatializing supply chain inventory and impacts associated with resource use, and more specifically water use, in heterogeneous agriculture production and trade. To illustrate the framework, we use a case study of milk production in the United States up to 'farm gate,' at which point milk is shipped for processing. Given the challenges of efficiently combining detailed process-based inventory data and impact assessment—without losing spatial information—we present an approach that occurs as a pretreatment step of the classical LCA calculation (using a technology matrix, etc.), avoiding issues of forcing computationally intensive calculations in LCA software or disaggregated (and duplicated) unit processes.[35] This approach is a matrix-based calculation focusing on the dominant production stages for the considered impact categories (here feed production and on-farm activities) that can be used as *input* to LCA software and databases to determine spatially explicit inventories and impact.[36] Indeed, the process and transport matrices presented here could be used to create and populate a full process-based MRIO matrix for the relevant activities. The outputs of this approach are geospatially meaningful inventory or impact factors for foreground processes, at an arbitrary aggregation level (e.g., state, watershed, or region) that can be used in a full Life Cycle Analysis. That is, the full LCA of crop production would account for background processes such as water use to produce fertilizer, water to produce energy for transport, etc.

The specific objectives of this work are the following:

1. Design a matrix-based framework to structure and track the spatial relationships between life cycle inventory (stemming from feed production, transport, and milk production) and impact (water stress).
2. Apply this matrix framework to the case of water use associated with spatially differentiated feed production and milk production in the United States.
3. Assess the variability and uncertainty associated with inventory and impact, demonstrating the importance of appropriately accounting for this spatial variability, even in the face of uncertainty.

This approach has direct applicability to life cycle assessment, but is also important for applications such as footprinting or tracking flows of goods.

■ MATERIALS AND METHODS

This section defines the case study system, relevant input data, and then develops the matrix-based spatial approach,

System Definitions and Underlying Data. An industrialized milk production system, such as that in U.S., can be characterized as follows: feed for dairy cows is produced using various resources and inputs (e.g., agricultural land, fertilizers, irrigation water). Feed is then transported to dairy farms, with transport distances varying between locally grown crops (e.g., silage grown directly on the dairy farm or transported short distances), regional crops (e.g., hay, possibly transported interstate), or nationally traded commodity crops (e.g., corn grain, soybean, and their byproducts). Thus, milk produced in one region of the country has typically used inputs from other regions.

In this study, we focus on the on-farm, consumptive water scarcity impacts for the production of feed crops and milk, up to dairy farm gate (i.e., not including water use in processing or consumer stages), which typically account for the majority of water use related to the full life cycle of milk consumption. The on-farm activities include feed consumption, washing of the barn and dairy parlor, and drinking water for cows. The present study addresses these main stages for water consumption in a detailed, spatialized analysis. This approach can be complemented by nonspatialized addressed upstream and downstream processes (e.g., water consumption associated with fertilizer

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CF: Characterization Factors (water stress)

$L_{eq.\,in\,competition}(i)/L_{consumed}(j)$

zone of water impact	zone of water use: HD	Med.	S	TR	Rest US
HD	1.0	-	-	-	-
Med.	-	0.97	-	-	-
S	-	-	0.90	-	-
TR	-	-	-	3.5E-2	-
Rest U.S.	-	-	-	-	0.30

B_{feed}: Emission (corn grain)

$L_{consumed}(i)/kg_{feed\,produced}(j)$

zone of water use	zone of feed production: HD	Med.	S	TR	Rest US
HD	1.0E+3	-	-	-	-
Med.	-	8.0E+2	-	-	-
S	-	-	2.2E+2	-	-
TR	-	-	-	10	-
Rest U.S.	-	-	-	-	36

$I_{feed}^{prod} = CF \times B_{feed}$ = Impact from production (corn grain)

$L_{eq.in\,competition}(i)/kg_{feed\,produced}(j)$

zone of water impact	zone of feed production: HD	Med.	S	TR	Rest US
HD	1.0E+3	-	-	-	-
Med.	-	7.8E+2	-	-	-
S	-	-	2.0E+2	-	-
TR	-	-	-	0.34	-
Rest U.S.	-	-	-	-	11

FT_{feed} Feed transport and trade (corn grain)

$kg_{feed\,produced}(i)/kg_{feed\,consumed}(j)$

zone of feed production	zone of feed consumption: HD	Med.	S	TR	Rest US
HD	0.30	-	-	-	-
Med.	-	0.19	-	-	1.2E-03
S	0.42	0.53	0.87	-	0.11
TR	-	-	-	0.51	5.1E-3
Rest U.S.	0.29	0.28	0.13	0.49	0.88

$I_{feed}^{cons} = I_{feed}^{prod} \times FT_{feed}$ = Impact from consump. (corn grain)

$L_{eq.in\,competition}(i)/kg_{feed\,consumed}(j)$

zone of water impact	zone of feed consumption: HD	Med.	S	TR	Rest US
HD	3.0E+2	-	-	-	-
Med.	-	1.5E+2	-	-	0.92
S	83	1.1E+2	1.7E+2	-	22
TR	-	-	-	0.17	1.7E-3
Rest U.S.	3.1	3.0	1.4	5.2	9
Total induced	3.8E+2	2.6E+2	1.8E+2	5.4	33

R_{feed}: Rations (corn grain)

$kg_{feed\,consumed}(i)/kg_{FPCM\,produced}(j)$

zone of feed consumption	zone of milk production: HD	Med.	S	TR	Rest US
HD	0.14	-	-	-	-
Med.	-	0.13	-	-	-
S	-	-	0.14	-	-
TR	-	-	-	0.16	-
Rest U.S.	-	-	-	-	0.14

$I_{milk}^{zone} = I_{feed}^{cons} \times R$ = Impact from milk prod. (all feed + barn)

$L_{eq.in\,competition}(i)/kg_{FPCM\,produced}(j)$

zone of water impact	zone of milk production: HD	Med.	S	TR	Rest US
HD	5.3E+2	-	16	-	3.1
Med.	-	2.9E+2	-	-	5.2
S	28	32	1.2E+2	-	5.3
TR	-	-	-	0.38	6.1E-4
Rest US	60	19	51	2.9E-2	64
Total induced	6.2E+2	3.4E+2	1.9E+2	0.41	78

$P_{milk}^{national}$: Milk production fractions (nat'l milk prod.)

(−)

zone of water impact	zone of milk production: HD	Med.	S	TR	Rest US
HD	0.02	-	-	-	-
Med.	-	0.22	-	-	-
S	-	-	0.01	-	-
TR	-	-	-	0.13	-
Rest U.S.	-	-	-	-	0.62

$I_{milk}^{national} = I_{milk}^{zone} \times P_{milk}^{national}$ = Impact from national milk prod. (all feed + barn)

$L_{eq.in\,competition}(i)/kg_{FPCM\,produced}(j)$

zone of water impact	zone of milk production: HD	Med.	S	TR	Rest US	Total endured
HD	12	-	9.0E-2	-	1.9	14
Med.	-	64	-	-	3.2	68
S	0.63	7.1	0.69	-	3.3	12
TR	-	-	-	4.9E-2	3.8E-4	4.9E-2
Rest U.S.	1.3	4.2	2.9E-1	3.7E-3	40	46
Total induced	14	76	1.1	5.2E-2	48	Total 1.4E+2

Figure 1. Set of simplified matrices for 4 different climate zones, hot and dry (HD), Mediterranean (Med.), steppe (S), temperate rain (TR), and the rest of the U.S. ("Rest U.S.") to determine the impact of corn grain (top half) and all feeds and on-farm activity (bottom) for milk production. Matrices are described in the text.

production) to produce a full life cycle approach. The quantities of produced or consumed feed are expressed on a dry matter basis (DM), and milk production is normalized to fat-protein-corrected milk (FPCM), using the approach of Thoma et al.,[37] which has been adopted by the International Dairy Federation.[38] In this paper, the term kg milk is often used for readability, though it refers to FPCM.

We consider the production of 12 main feeds:[39] alfalfa hay, alfalfa silage, corn grain, corn silage, distiller's dry grains (DDGS) dry, DDGS wet, grass hay, grass pasture, grass silage, soybean, soybean meal, and a feed mix. The first 11 feeds represent approximately 83% of the ration mass, with slight variations depending on the region. The remainder was modeled as a feed mix comprised of corn and soybeans. The fraction of corn grain (0.61) and soybean (0.39) in the mix was based on an analysis of the dominant contributions to the components of the feed mix (see Supporting Information (SI), Section 1.2).

All data on crop yields, irrigation, feed transport, rations fed to livestock, and milk yields were gathered from publicly available data[40,41] and from survey information that was carried out in a milk greenhouse gas study.[37,42] That survey divided the

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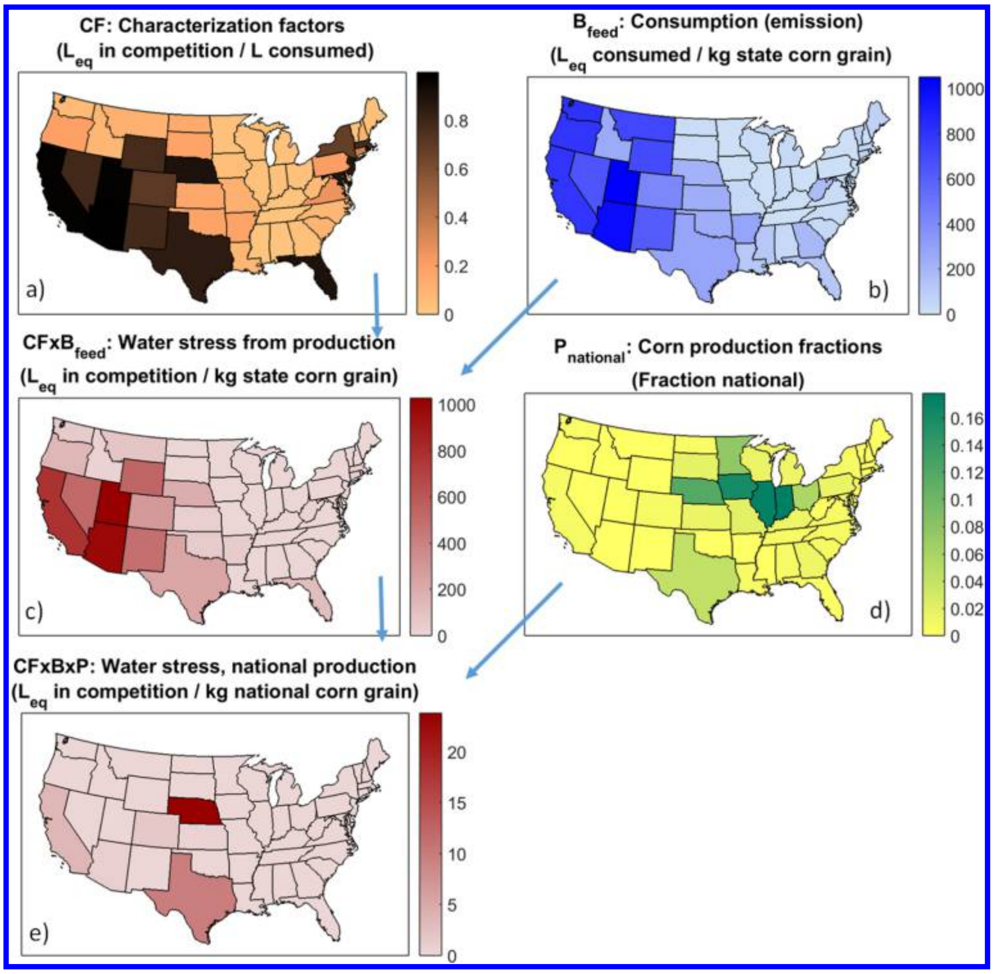

Figure 2. Spatialized matrix calculation determination of water stress impact of corn grain production in the U.S.

U.S. into five milk-producing regions, based on climate and dairy practices (see SI, Section 1). Feed transport was assumed to be intrastate (silages), intraregional (hays), or intranational (corn, soy, and their byproducts) (see SI, Section 1.4). The relationship between quantities of irrigation water and the consumptive water use is discussed in SI, Section 1.3. See SI Section 1 for more information about input data, including the allocation between milk and beef, and the System Definitions and Underlying Data section for a discussion of input data uncertainty.

Impacts are assessed using the water stress index (WSI), a logistic function ranging from 0 to 1 that corresponds to a ratio of water withdrawals to water availability, adjusted for a climate-based variation factor.[20] Thus, this index is the life cycle characterization factor used to translate inventory (environmental interventions) to impact. WSI factors were provided at a $0.5 \times 0.5°$ resolution and aggregated to states or watersheds (HUC-2, Hydrologic Unit Code level 2[43]) in ArcMap by overlaying HUC-8 estimates of dairy cow population,[8,40] the 0.5° WSI grid cells, and the state or watershed boundaries, performing a geometric intersection of the polygons, and calculating an average, weighted by area and dairy cow population, of resulting polygons within the desired aggregation level. Water stress is expressed as "liters equivalent in competition" ($L_{eq\ in\ competition}$), and the impact (or characterization) factors relate consumptive water use to this stress. See Pfister et al.[34] for a discussion of differences between consumption and stress.

Matrix Approach to Track Spatial Inventory, Trade, and Impacts. In this section, we describe the matrix approach for the national water use impact assessment of milk production.

Formalization of the Matrix Approach. The above-described process can be structured and implemented through a series of matrices representing water stress, water consumption, feed rations for dairy, feed trade within the U.S., and milk production. These matrices could be scaled to any resolution, with this work focusing on state resolution for inventory and HUC-2 watershed resolution for impact (see SI, Section 4). The matrix approach and its intermediate calculations are described below, beginning with example of a single feed and overall milk production. As noted above, the overall dairy ration is a mix of a variety of feeds. Results for each feed and on-farm activity (e.g., drinking water for cows) are combined for total water impact. Calculations were performed in Matlab, generating overall inventory and impact matrices that could be imported into standard LCA software (e.g., SimaPro)

Figure 1 and the following text present an example of the water impacts of milk production related to corn grain feed and national milk production, modeled with a reduced matrix of five zones corresponding to different climate zones found in the U.S.: hot and dry (HD), Mediterranean (M), steppe (S), and temperate rain (TR) (examples of states with these characteristics are Arizona, California, Nebraska, and Wisconsin, respectively). The last zone, named "Rest U.S.," represents

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the remainder of the United States, using corn grain or milk production-weighted averages, where appropriate. For example, the *CF* matrix uses state CFs for the five sample regions, and the "Rest U.S." *CF* is an average weighted by milk production. The upper half of the figure is for corn grain, whereas a horizontal line separates milk-related matrices (I_{milk}^{state}, P_{milk}^{milk}, $I_{milk}^{national}$) at the bottom. Figures 1 and 2 show similar data from different perspectives: the former presents representative and aggregated values, while the later highlights the spatial distribution of the full data set, including the intersection between states with water scarcity and with high corn production.

Feed Production Impact Matrix. To first assess the impact of feed production, we multiply an environmental inventory matrix (B_{feed}) by a characterization factor matrix (CF) to obtain the impact matrix (I_{feed}^{prod}) for the specific feed studied (e.g., corn grain in Figure 1):

$$I_{feed}^{prod} = CF \times B_{feed} \qquad (1)$$

Where I_{feed}^{prod} ($L_{eq\ in\ competition}/kg_{feed,produced}$) is the impact matrix of feed production, expressing the water stress in row I per kg DM feed produced in column j. B_{feed} ($L_{consumed}/kg_{feed,produced}$) is the inventory matrix for given a feed, expressing the liters consumed in location i from production of 1 kg DM feed in location j. CF ($L_{eq\ in\ competition}/L_{consumed}$) is the characterization factor matrix, expressing the water stress in location i per liter water consumed in location j.

As shown in Figure 1, the irrigation requirements (B matrix) show high variations, between 10 to 1000 L consumed per kg corn grain, and are then multiplied with the local water stress *CF* matrix, which also covers a wide range of values, from 0.03 to 1. This multiplication yields variable impacts in the I_{feed}^{prod} matrix, with 1000 $L_{eq\ in\ competition}/kg_{corn,produced}$ in the hot and dry, versus only 0.3 $L_{eq\ in\ competition}/kg_{corn,produced}$ in the temperate rain zone.

In this example, the associated inventory is consumption of water, but the B matrix could also be emissions, for example, of pesticides or nutrients. Furthermore, in this case study, the B matrix is a diagonal matrix (feed production in state i corresponds to water consumption in state i), but if water were transported from one state to another, it would be possible to track inventory associated with locations other than location of production. In the case of water stress, the *CF* matrix is diagonal: impact occurs in the location of consumption.[20] For other impact categories that may involve environmentally mediated transport of substances, such as eutrophication, impacts are not restricted to the location of an emission (e.g., emissions of nitrogen in the Mississippi river basin contribute to eutrophication in the Gulf of Mexico), and a nondiagonal *CF* matrix would capture the relationship between the location of an emission and its impact.

Feed Consumption Impact Matrix. To assess the impacts of feed consumption, we multiply the I_{feed}^{prod} matrix by the FT_{feed} matrix:

$$I_{feed}^{cons} = I_{feed}^{prod} \times FT_{feed} \qquad (2)$$

where I_{feed}^{cons} ($L_{eq\ in\ competition}/kg_{feed,consumed}$) is the impact matrix for consumption of the feed, expressing the water impacts in location j due to consumption in location i. The sum of each column of this matrix is the total impact in location j due to consumption in the other locations i. FT_{feed} ($kg_{feed,produced}/kg_{feed,consumed}$) is the feed trade matrix, expressing the kg feed produced in location j per kg feed consumed in location i. The FT_{corn} matrix is the feed trade matrix that indicates the provenance of corn grain consumed in each zone. (The FT_{feed} matrix varies for each feed crop; see SI Section 1.4.) In Figure 1, the Mediterranean zone produces 19% of the corn grain consumed in that zone, with the remainder from the steppe zone (53%) and the rest of the U.S. (28%); the temperate rain and hot and dry regions do not supply any corn grain to the Mediterranean zone, even though they produce it (e.g., the hot and dry zone supplies 30% of its own corn grain). As observed by comparing the I_{feed}^{cons} and I_{feed}^{prod} matrix, feed transport tends to reduce the variation in water impact per kg consumed feed between states, since consumption of corn from the corn belt, which supplies a large fraction of the country's corn grain, also implies that the consuming regions' water impacts are proportionally influenced by the water impacts in the corn belt.

Milk Impact Matrix. To model the impact of milk production per kg milk produced, we combine the feed consumption impacts described above with specific rations in each state (R_{feed} matrices), summed across all feeds (n_{feed} is the total number of feeds considered, in this case, 12) and also including water used on farm for washing and drinking:

$$I_{milk}^{location} = \sum_{feed=1}^{n_{feed}} (I_{feed}^{cons} \times R_{feed}) + I_{farm} \qquad (3)$$

Where $I_{milk}^{location}$ ($L_{eq\ in\ competition}/kg_{FPCM,produced}$) is the water impact in (row) location i per kg FPCM production in (column) location j due to the consumption of all feeds and farm activities. The spatial extent of locations is set by previous matrices or an intermediate transformation matrix. R_{feed} ($kg_{feed,consumed}/kg_{milk,produced}$) is the diagonal matrix of the ration for a given feed, expressing the kg feed consumed in each location i per kg milk. R_{feed} is kept as a diagonal matrix rather than a vector to keep information on feed provenance in subsequent calculations. I_{farm} ($L_{eq\ in\ competition}/kg_{FPCM,produced}$) matrix, is the impact matrix for dairy farm activities, and is the product of $CF \times B_{farm}$, which is analogous to eq 1. B_{farm} expresses L consumed for washing and drinking in location i per kg milk produced in location j. (I_{farm} and B_{farm} are not shown in Figure 1.)

Dairy cow diets vary across the U.S.: in our example that focuses on the contribution of corn grain only, cows in the temperate rain zone eat more corn grain per kg milk produced (0.16 kg corn grain/kg milk) than cows in the Mediterranean zone (0.13 kg corn grain/kg milk). In Figure 1, since the hot and dry zone sources corn grain from itself and the also water stressed steppe, it has the highest impact overall. The temperate rain zone, on the other hand, sources corn grain from itself and the rest of the U.S., where water stress is low, resulting in low water impact associated with milk production in that zone. The vector created by summing along columns of $I_{milk}^{location}$ represents the total impact from producing 1 kg milk in each zone (columns) with variations in water impact of milk due to corn grain, from over 600 $L_{eq\ in\ competition}/kg_{milk,produced}$ for the hot and dry zone to less than 1 $L_{eq\ in\ competition}/kg_{milk,produced}$ for the temperate rain zone.

The $I_{milk}^{location}$ matrix also shows the location of impacts due to milk production in each zone. For example, a significant fraction of impact from milk production in the Mediterranean zone takes place in the same location (290 $L_{eq\ in\ competition}/kg_{milk,produced}$), but the steppe zone also endures a part (32

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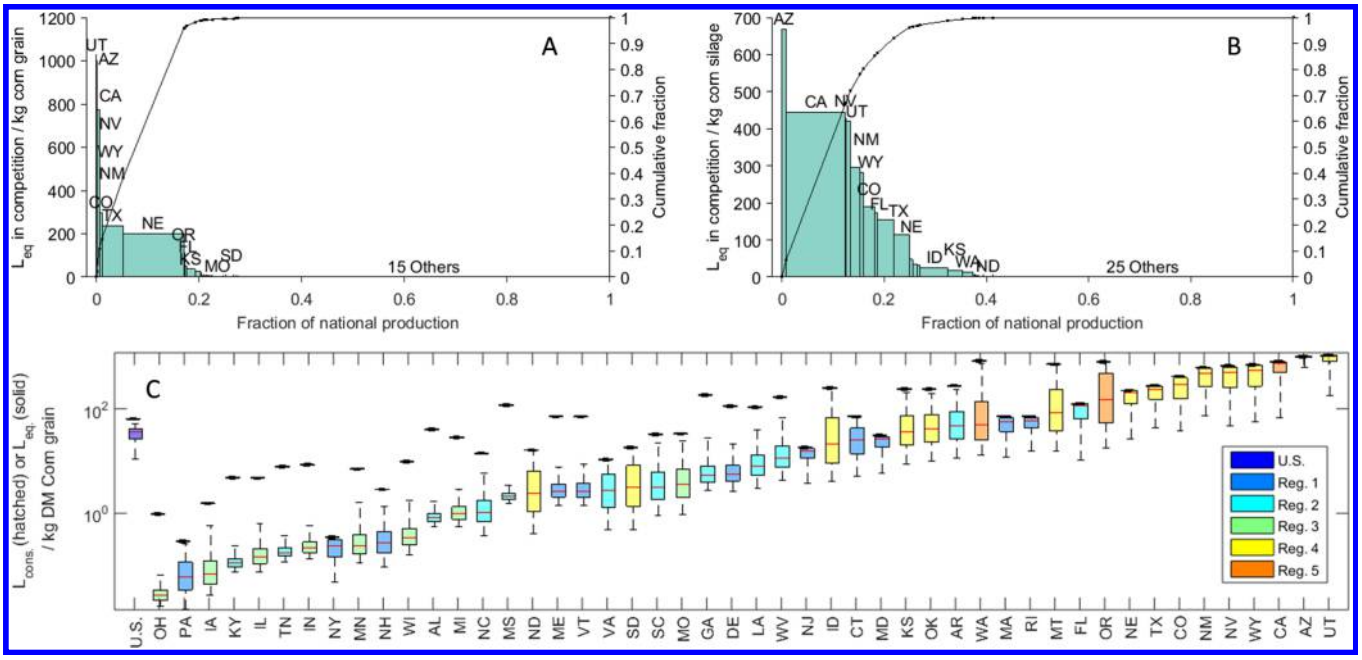

Figure 3. Water deprivation impact per kg (a) corn grain and (b) corn silage as a function of the contribution of each state to national production (Right Y scale: cumulative fraction of the water deprivation). Panel (c): state-based water consumption (top values, hatched) and water stress impact (bottom values, solid) for corn grain production in each state, with error bars indicating 95% confidence. Values are ranked by increasing median water impact, and states are colored according to their region.

$L_{eq\ in\ competition}/kg_{milk,produced}$) of the impacts induced by production in the Mediterranean region.

National Inventory and Impact of Milk. Finally, to calculate a matrix representing each state's contribution to the average water stress per kg national milk, we multiply the state $I_{milk}^{location}$ matrix by the national production matrix ($P_{milk}^{national}$), whose diagonal elements represent the fractional contribution of each zone to overall production:

$$I_{milk}^{national} = I_{milk}^{location} \times P_{milk}^{national} \quad (4)$$

where $I_{milk}^{national}$ ($L_{eq\ in\ competition}/kg_{milk,produced}^{national}$) is the impact of national milk production, with each matrix element expressing impacts in location i (row) due to milk production in location j (column). $P_{milk}^{national}$ (unitless) is the national production matrix (kept as a diagonal matrix rather than a vector to trace both induced and endured impact by location), expressing fractional breakdown of national milk production at the level of analysis (in this case, watershed).

The $I_{milk}^{national}$ matrix makes it possible to sum impacts induced elsewhere by production in a given location, or determine other locations' contributions to impacts endured in a given location. The sum of the columns of $I_{milk}^{national}$ represents the induced impacts by milk production in each state to the national average milk production impacts, with, for example, the largest contribution of 64 $L_{eq\ in\ competition}/kg_{milk,produced}$ national milk occurring in the Mediterranean zone out of a total of 140 $L_{eq\ in\ competition}/kg_{milk,produced}$. The sum of the rows represents the contribution of endured impacts in each state to the national average milk production impacts. The steppe zone, despite producing only 1% of national milk, endures 8.5% (12 $L_{eq\ in\ competition}/kg_{milk,produced}$ out of 140) of total national water stress.

The matrix approach is flexible, enabling the analysis of spatially varying inventory and impacts. Intermediary matrices can be used to further understand the contributions to each part of the production system. For example, omitting the *CF* matrix provides inventory data directly, such as the water used per kg milk produced in a given zone ($B_{feed} \times FT_{feed} \times R_{feed}$). Alternatively, adding national production at the feed level shows the contribution of each state to the national impact of corn grain per kg national corn produced ($CF \times B_{corn} \times P_{corn}^{national}$, where $P_{corn}^{national}$ is the respective fraction of corn grain feed production in each watershed or state. Intermediate matrices can be used to transform the spatial resolution of data (see SI, Section 4).

In this study, the spatialized matrix approach focused on agricultural production stages. To extend to a full life cycle perspective, impacts of the supply chain with unknown locations (e.g., fertilizer production or the milk processing facilities) can be added to the total impacts of state, watershed, or national milk to provide overall impacts.

Uncertainty Assessment. Uncertainty estimates for inventory data are available from the ecoinvent database and the U.S. milk GHG study.[37,42,44] This uncertainty is comprised of uncertainty in collected data, as well as additional uncertainty due to the data pedigree (see SI Section 2.1). We have estimated overall uncertainty for the spatially modeled field and farm gate data presented here, considering contributions from the water to availability ratio, the temporal variability factor, and the functions used to create the WSI, as described in SI Section 2.2 (see also Pfister and Hellweg[45]). For both inventory and impact data, positive values bounded by zero are expected, so uncertainty was assumed to be lognormally distributed. Uncertainty is expressed as a squared geometric standard deviation (GSD_{95}^2), indicating that 95% of the data fall within the geometric mean multiplied by the GSD_{95}^2 and the geomean divided by the GSD_{95}^2. Uncertainty calculations were performed in Matlab using Monte Carlo analysis ($n = 1 \times 10^6$), representing a random sample from the corresponding log-normal distribution (median and GSD_{95}^2). These vectors

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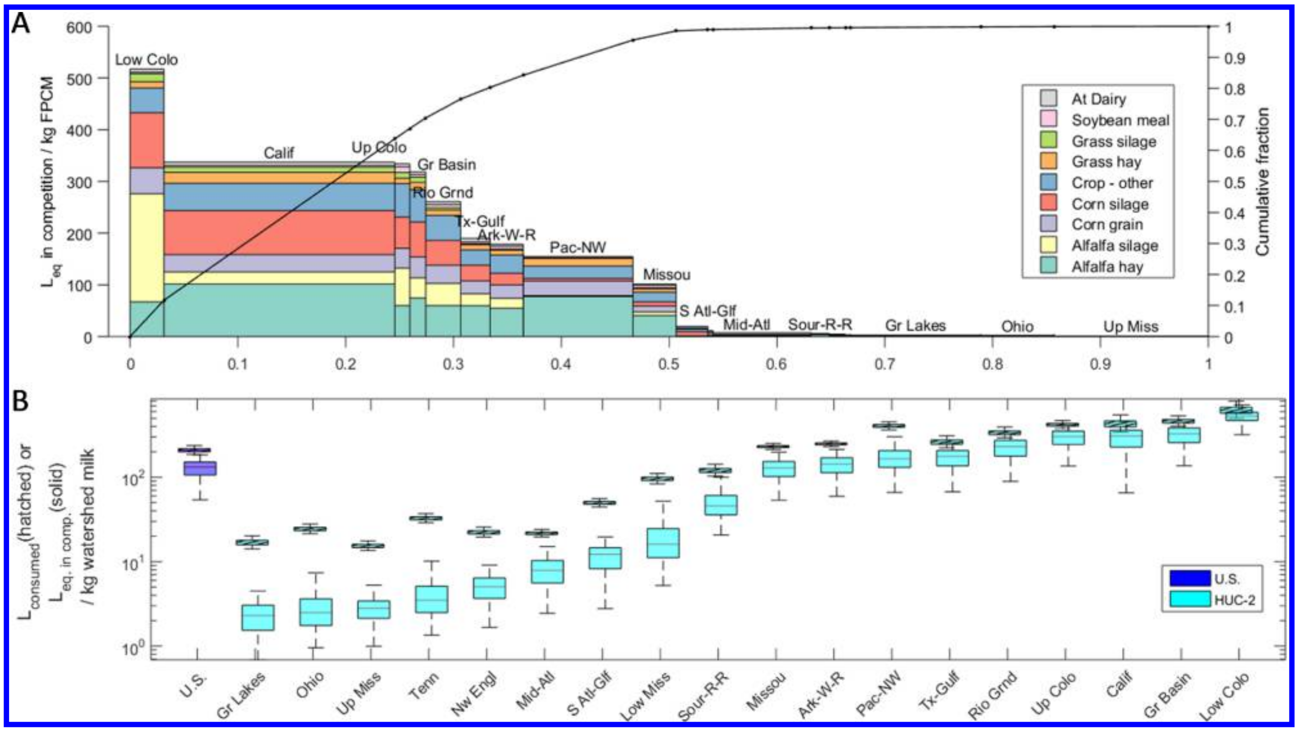

Figure 4. a) Water deprivation impact per kg watershed milk produced as a function of the contribution of each watershed to national production, differentiated by feed and on-farm activity ("At Dairy"). Right Y scale: cumulative fraction of the water deprivation impact per kg national milk produced. b) Water consumption (top values, hatched) and water impact (bottom values, solid) for each watershed, with error bars indicating 95% confidence.

were generated again when uncertainty was independent, and reused for nonindependent variables.

RESULTS AND DISCUSSION

This section presents the results of the national model for feed production, using the example of corn grain, and then the water impact associated with milk production at watershed and national level.

Impacts of Feed to Farm Gate. Figure 2 presents the combination of the elementary data and the path for obtaining the final impact per kg corn grain produced at the national level ($kg^{prod}_{US\ corn}$).

Figure 2b) illustrates the water consumed per kg DM corn grain produced in each state. Combined with the characterization factors for WSI ($L_{eq\ in\ competition}/L_{consumed}$)[20] in Figure 2a), we obtain the water stress per kg corn grain produced in each state (Figure 2c). There is a strong correlation between irrigation requirements (2a) and WSI (2b), both because of water availability and possible demands from other sectors. The water deprivation impact per kg corn grain produced in each state is weighted by the fraction of national corn grain produced (2d) to calculate national corn grain water deprivation impact, as shown in (2e). As a result, only states with both significant corn grain production and non-negligible water stress contribute substantially to the national value, the highest contributions coming from Nebraska and Texas.

The contribution of each state to the water impact of corn grain can also be represented in using a variable width bar graph (Figure 3a). Corn silage is shown in Figure 3b.

In Figure 3a and b, the state fraction of the national corn grain and corn silage production are represented on the *x*-axis. The water impacts per kg corn produced in each state are represented on the *y*-axis. As a result, the area associated with each state represents that state's contribution to the national water impacts for corn production. The sum of the areas represents the total impact of national production. For corn grain (Figure 3a), the national total is 41 $L_{eq\ in\ competition}/kg^{national}_{corn,\ produced}$. This total is dominated by Nebraska and Texas. Nebraska does not have the highest impact per kg corn grain, but, due to its relatively large share in national production (11%), it is the first contributor in the national impact (58%). Most of the corn belt states have high production but low water deprivation impact.

For corn silage (Figure 3b) the total impact of national corn silage production is 85 $L_{eq\ in\ competition}/kg^{national}_{corn\ silage,\ produced}$. California represents 60% of this impact (51 $L_{eq\ in\ competition}/kg_{corn\ silage}$); this is due to a combination of a higher water stress index, and a relatively large share within the national production of corn silage (12%), as silage is grown as feed for the dairy cows in that state. The comparison of corn grain and corn silage emphasizes the importance of production amounts and conditions, demonstrating the importance of considering spatial differentiation with respect to water.

Figure 3c shows the uncertainty and variability related to the state values of corn grain shown in Figures 3a (similar figure for corn silage production in SI Section 2.1). Water consumption and water impacts per kg dry matter state-based corn produced are shown on the *y*-axis (note logarithmic scale). On the horizontal axis, states are ranked by increasing median water stress to produce corn grain, and states are colored according to their region. The uncertainty on the inventory (water consumption) is clearly modest (a $GSD_{95}{}^2$ typically less than 1.6) relative to the uncertainty on the impact (overall $GSD_{95}{}^2$ values of five or greater, with the largest contribution from water availability; see SI Section 2.2). We see the highest stress in Western states (region 4 and 5), and the lowest in Midwest

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(region 3). Furthermore, the confidence intervals allow one to distinguish between uncertainty and meaningful variability (e.g., a state with a lower bound at 10 $L_{eq\ in\ competition}$/kg milk is different than a state with an upper bound at 1 $L_{eq\ in\ competition}$/kg milk).

Milk Production. Summing over feeds and on-farm water use, the national average water consumption associated with milk production is 210 $L_{consumed}/kg^{national}_{milk,\ produced}$, and is dominated by feed irrigation. When the calculation is taken to impact (eq 4), the average national water deprivation is 130 $L_{eq\ in\ competition}/kg^{national}_{milk,\ produced}$, which is largely due to feed production (96%), with dairy farm water use for washing and drinking representing the remainder. Figure 4 presents these national results for milk as a variable width graph (top portion), and with uncertainty for each watershed and the U.S. (bottom).

In Figure 4a, we see that western milk-producing watersheds such as the Upper and Lower Colorado, California, Pacific Northwest, and Great Basins are the dominant contributors (82%) to the total water impact, with a combination of water stress above 300 $L_{eq\ in\ competition}$/kg milk and production of ~28% of U.S. milk. Watersheds in areas with lower irrigation requirements (beginning with the Atlantic watersheds and moving to the right) contribute approximately 50% of national milk production but account for less than 1% of water impact. At the feed level, alfalfa hay, alfalfa silage and corn silage dominate the impact, representing 23%, 22%, and 19% respectively, as these locally or regionally produced feeds may require irrigation in western areas. The nationally traded commodities such as soybean and corn grain have a lower share of the total impact, as they are largely produced in areas with lower irrigation demands.

Figure 4b shows the uncertainty and variability related to the water consumption and stress of milk in each state, ranked by increasing median water stress. As was the case for corn grain, the uncertainty on the water consumed is clearly modest relative to the uncertainty on the water impacts, and the spatial variability can be greater than uncertainty. The water stress in Western watersheds (beginning at the Missouri and moving to the right, median values are >100 $L_{eq\ in\ competition}$/kg milk) is significantly higher, at the 95% confidence level, than it is in the Great Lakes and Mississippi water basins, many of which are <10 $L_{eq\ in\ competition}$/kg milk.

■ DISCUSSION

Importance of Spatial Differentiation. For water impact, the spatialized implications of feed production and trade are critical. Water impacts are very dependent on local conditions, and vary by several orders of magnitude across the U.S. Accounting for variability in WSI as it affects local crops (as opposed to applying an average *CF*) is critical, as it captures the importance of areas with low water availability (which is connected to irrigation demands) and non-negligible milk production. At a national level, the spatialized analysis results in a geometric mean of 130 $L_{eq\ in\ competition}/kg^{national}_{milk,\ produced}$, with 95% confidence interval from 54 to 180 $L_{eq\ in\ competition}/kg^{national}_{milk,\ produced}$. If one uses the average U.S. water scarcity index of 0.50 $L_{eq\ in\ competition}/L_{consumed}$ reported in Pfister et al.,[20] the overall U.S. water stress is 73 $L_{eq,\ in\ competition}/kg^{national}_{milk,\ produced}$ (see SI Section 3). This average result underestimates the median of the national spatial calculation by approximately a factor of 1.8 but is within its 95% confidence interval. This factor is larger than the uncertainty on inventory data (see SI Section 2.1).

Variability vs Uncertainty. This study is one of the first to systematically integrate uncertainty and spatial differences for inventory data (the consumption of water resulting from, e.g., reported irrigation, feed trade, the ration, and milk yield) and impacts (accounting for water resource variability factors, human regulation of flows, and uncertainty related to modeling). The challenge presented by the heterogeneous U.S. is to capture these differences systematically in a multicomponent system, allowing for meaningful differences to be identified. Figures 3c and 4b show a modest uncertainty in inventory but a much larger uncertainty in impact. This relationship probably holds for other impact assessment categories, although it is not estimated in most LCAs. By quantifying the uncertainty, this analysis shows that the water impact associated with milk production does have meaningful differences between areas of production. Without separating variability and uncertainty, uncertainty may be artificially increased via an implicit combination of the two.

Flexibility of the Spatialized Matrix Approach. The approach presented in this paper enables the analysis of results at intermediate levels and the differentiation of induced versus endured impacts. The resolution can be adjusted, depending on the available data: in this case, the inventory was at the state level. The analysis was moved to watershed level in the *CF* matrix, enabling presentation of impact results in a spatial format consistent with the impact category (see SI, Section 4).

In this article, the water for feed production in a given state is consumed in that same state; in the matrix approach, this means that the B matrix is diagonal. Introducing a nondiagonal B matrix would enable to account for transport of water from one location to another. This could become important at higher resolution or if a large interstate water transfer were developed.

Similarly, the water impact assessment methodology currently assumes that the impact from water consumed in a given watershed occurs in the same watershed; in the matrix approach, this means that the *CF* matrix is diagonal. A nondiagonal *CF* matrix could account for further development in water impact assessment methods, should they capture downstream impacts of water withdrawal. A nondiagonal matrix would also be used in cases where a transport mechanism (e.g., aquatic or atmospheric) caused impacts in locations different than the emission location. The approach presented here is flexible and could be extended to more complex product systems, provided data are available (finding consistent data across countries, for example, may be a challenge). Results from this approach can be integrated into other analyses, as described above.

Data Quality Improvement. While this study improves understanding of water impacts related to livestock feed and dairy production, underlying data improvements could reduce uncertainty in the assessment. Given the ranges of uncertainty in impact vs inventory, reductions in impact uncertainty with method development will yield the most benefit in terms of overall uncertainty. In the case of inventory, the following warrant further study:

Improve Resolution, Especially in Critical States. In this study, the lowest resolution is the state; states have been assumed to be homogeneous for irrigation requirement and water stress. However, in some cases, like Nebraska or California, there are intrastate climate and irrigation differences, for example, between eastern and western Nebraska or between Northern and Southern California. In those cases, it would be useful to refine the resolution at the inventory level (i.e.,

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irrigation data per county or per subwatershed instead of per state) in order to target areas for, e.g., irrigation improvements.

Improve Feed Trade Data. Based on conversations with dairy and feed producers, we have classified feeds as locally, regionally, or nationally produced. Locally produced feeds are defined by state yields and irrigation, and regionally are assumed to be traded freely within the five U.S. regions. Given the importance of the silages and hays in the overall assessment, it would be worthwhile to conduct a more detailed study of production of those feeds, particularly in states with high dairy production. Furthermore, due to the increasing share of corn grain used for biofuel production, it may be useful for interstate trade data to distinguish between corn grain used for biofuel and other corn grain.

Feed Mix and Water Requirements. In the composition of the rations, the first 11 feeds capture approximately 83% of the ration; the remainder is made up of an assortment of feeds in very small proportions; however, many are corn or soy based (e.g., corn grain is 36% of concentrates[39,42]). Because corn and/or soybean tend to have non-negligible contributions to the various impact categories, the same is true for the feed mix. In a future study, refinement of the feed ration data will be useful.

Trade-off with Other Impact Categories. In water deprived regions, the use of irrigation, while having significant impact on water deprivation, induces higher yields. Those higher yields might reduce other environmental impacts (e.g., land use and terrestrial biodiversity) per kg feed produced. Therefore, beyond water deprivation impact, it is important to consider other environmental impact categories to have a more holistic assessment of any system, preventing any unintentional trade-offs.

■ ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge on the ACS Publications website at DOI: 10.1021/acs.est.6b04713.

> Temporal variability of inventory data, uncertainty approaches for inventory and impact, examples of aggregation to watershed, and a comparison with nonspatial calculations (PDF)

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Notes

The authors declare no competing financial interest.

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