

Characterization of Uncertainty and Variability of
Freshwater Consumption Impacts in Life Cycle Assessment

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Abstract

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Life cycle assessment (LCA) provides a standardized protocol for estimating a wide range of life cycle technology impacts. LCA is used to make comparisons between alternative technology systems and to identify opportunities for reducing environmental impacts at the local, regional, and global scales. Until recently freshwater as a resource has been neglected from LCA studies. However following record draughts and massive agricultural losses in recent years, the use of LCA, or life-cycle type approaches, have been suggested as a way to identify situations of high water use and possible alternative technologies to reduce water scarcity impacts. Several methods have been proposed in the literature for estimating freshwater consumption impacts—although varying in their overall approach and goal, the distinction between, and quantification of, freshwater use and consumption is common to all methods. Freshwater use refers to any freshwater for which some productive use has been made, and may or may not be available at its origin for further use by other water users. Freshwater consumption refers to freshwater use that is no longer available to other users, such as through evaporative losses. The importance of this distinction is

that consumed freshwater can contribute to resource scarcity, unconsumed water that has been used can be recycled and does not contribute to scarcity. Also common to all methods in the literature is the lack of analysis of uncertainty and variability in the estimation of freshwater consumption. This work demonstrates the importance of uncertainty and variability characterization in Life Cycle Assessment, using the study of freshwater consumption for a crop production unit process as an example.

A sensitivity analysis and uncertainty analysis is performed on the estimation of two classes of freshwater consumption impacts at the farm level spatial scale: green and blue water (abbreviated as GW and BW respectively). Green water refers to the amount of water consumed that originated as local rainfall, blue water refers to the amount of water consumed that was abstracted from surface or groundwater sources. Thus, in the context of crop production green water is a function of land use and blue water is a function of the amount of irrigation water applied. It is found that green water is most sensitive to precipitation and rate of crop water uptake, with estimates range from $\pm 20\%$ and $\pm 18\%$ of the estimate respectively. Neglecting sparse environmental data such as wind speed and relative humidity can introduce uncertainties of up to 30% of the estimate. Uncertainty in blue water consumption is driven by the amount of irrigation water applied. For cases of under irrigation, uncertainty in blue water consumption is equal to uncertainty in the water application data and averages 18% of the estimate. For cases of over irrigation, the uncertainty in blue water consumption is equal to the uncertainty in green water consumption. For cases of irrigation application matching the crop water demand, the uncertainty compounds, and is equal to 40% of the estimate on average.

Through a process known as atmospheric recycling, evaporated water can return to the terrestrial ecosystem as precipitation within days or weeks of having entered the atmosphere, reducing the impact of freshwater consumption. Variability associated with temporal and spatial scales and with boundary selection has a substantial impact on the magnitude of the freshwater consumption impacts, but the consideration of these control volume issues has not been considered in the literature in the context of freshwater consumption impacts in LCA. A bounding analysis is performed to determine the effect of atmospheric recycling uncertainty has on freshwater consumption impacts. Atmospheric recycling can reduce the impact of freshwater consumption from 0 to 80% of the farm level estimate, depending on the region, spatial scale, and temporal scale considered within the control

volume. In addition there exists unquantified uncertainty associated with how changes in land cover will effect precipitation, irrigation response, and associated freshwater consumption impacts in the context of LCA.

Energy required for irrigation is estimated, specifically for water withdrawal from surface and groundwater sources, and water application by pressure and gravity irrigation systems. It is shown that the energetic cost of water withdrawal and application is higher in regions experiencing freshwater scarcity. It is suggested that further research into the interdependence of water and energy production, known as the water-energy nexus, be considered as an alternative approach to currently proposed freshwater impact characterization methods. It is argued that, although uncertainty associated with energy use for irrigation can as high as 40% of the estimate, particularly for groundwater extraction in areas under water stress, it can be bounded as opposed to the unbounded uncertainty associated with atmospheric recycling.

The following files are included with this dissertation as supporting information:

- cumulative_plots.zip – contains the plotted results of the Monte Carlo estimates for green and blue freshwater consumption.
- Supporting_information_1.xlsx – contains summary statistics for freshwater characterization factors and data and results for energy estimates for irrigation.
- Supporting_information_2.xlsx – contains input data for green and blue water consumption characterization factors.

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1. Introduction

Life cycle assessment (LCA) provides a standardized protocol for estimating a wide range of life cycle technology impacts (International Organization for Standardization 2006). LCA is used to make comparisons between alternative technology systems and to identify opportunities for reducing environmental impacts at the local, regional, and global scales. Examples of global scale impacts include contributions to climate change and ozone depletion; regional scale impacts include contributions to acid precipitation and impacts on water quality and freshwater availability; and local impacts include threats to human and ecosystem health. Additionally, LCA is being used to support regulatory decision making, notably in the United States as a means of quantifying and reducing greenhouse gases associated with the life cycles of biofuels within the context of the Renewable Fuels Standard within the US 2007 Energy Independence and Security Act (EISA 2007)¹. Thus, with the mainstream recognition of LCA as an effective environmental assessment technique comes the increased need to produce reliable, repeatable, and meaningful results.

Until recently freshwater as a resource has been neglected from LCA studies. However following record droughts and massive agricultural losses in recent years, the use of LCA, or life-cycle type approaches, have been suggested as a way to identify situations of high water use and possible alternative technologies to reduce water scarcity impacts. Also, water use and water resources are closely tied to energy production and use, known as “the water-energy nexus”. At the nexus, water is required to produce power, and power is required to transport water. Also, whereas in some cases the use of water means that water becomes unavailable for other purposes, other uses return water to the environment so that it remains available. Research supporting the debate as to how to operationalize water scarcity impacts have become commonly known as “water footprints”. Research in water footprinting is emerging (Arjen Y Hoekstra and Mekonnen 2012) and has spurred niche consulting services², on-line calculation tools³, and standards development efforts by the International Organization for Standardization (“ISO/DIS 14046 - Environmental Management -- Water Footprint -- Principles, Requirements and Guidelines” 2013). Despite these advances, there still lacks an agreed upon approach for quantifying water use and the impacts of industrial activities on water resources within the context of LCA.

¹ See <http://www.epa.gov/otaq/fuels/renewablefuels/index.htm>

² See <http://www.quantis-intl.com/waterfootprint.php>

³ See http://www.waterfootprint.org/?page=cal/waterfootprintcalculator_indv

One often neglected component of LCA is the estimation of uncertainty and its influence on the results of comparisons between alternative technologies. In their estimate of uncertainty in the life cycle greenhouse gas emissions of gasoline production, Venkatesh et al. note that “Previous analyses using deterministic emissions estimates to design policy targets dismiss its inherent uncertainty as either negligible or as difficult to deal with and hence largely tend to ignore its implications...” (Venkatesh et al. 2011). The authors find that for California’s low carbon fuel standard, both the deterministic baseline and the emissions reduction target fall within the 90% confidence interval of the baseline’s uncertainty, raising questions concerning the feasibility of enforcement of the policy as written. Implications associated with neglecting uncertainty extend beyond greenhouse gases to any study used to make comparisons between alternatives.

This dissertation reviews outstanding issues surrounding water footprinting in LCA including uncertainty associated with water footprint estimates, and explores some of the implications of these issues in the context of field crop production. Based upon the results, this dissertation outlines recommendations for future research. For the quantification of any life cycle impact, the ISO 14040 LCA standards define four distinct research phases: Goal and Scope Definition (GSD), Life Cycle Inventory (LCI), the Life Cycle Impact Assessment (LCIA), and the Interpretation phase. Each phase is described as follows.

1.1 Goal and Scope Definition

During GSD, the goal of the LCA is defined by identifying the intended application, the motivation for the study, the intended audience, and intended use of the LCA results (such as process improvement or technology comparison). Based upon the goal, the scope of the study specifies the functional basis for comparing technologies (called the functional unit of the study), the system boundary (a list of the life cycle processes to be modeled), the impacts to be considered, and the method for assessing impacts. For example, consider an LCA intended to compare a biofuel and a conventional petroleum derived fuel (Figure 1, left). The motivation of such an LCA might be to qualify the biofuel for sale under the 2007 Energy Independence and Security Act⁴, the intended audience

⁴ The 2007 Energy Independence and Security Act Section 526 specifies that “No Federal agency shall enter into a contract for procurement of an alternative or synthetic fuel, including a fuel produced from nonconventional petroleum sources, for any mobility-related use, other than for research or testing, unless the contract specifies that the lifecycle greenhouse gas emissions associated with the production and combustion of the fuel supplied under the contract must, on an ongoing basis, be less than or equal to such emissions from the equivalent conventional fuel produced from conventional petroleum sources.”

might be military purchasing agents, the functional unit might be a MJ of fuel, and the contribution to climate change would be the impact of interest. The system boundaries would include all processes needed for the production of the biofeedstock through fuel production and use as well as the life cycles of any resources used or waste management processes therein. Finally, specifying the use of impact methods from the Intergovernmental Panel on Climate Change (IPCC) defines and identifies the greenhouse gas (GHG) emissions to be accounted and assessed in the LCA.

Refer next to the figure on the right in Figure 1; the intent of the LCA would be to compare a biofuel and a conventional petroleum biofuel on the basis of freshwater use. In this case, the motivation of such an LCA might be to understand freshwater use for the biofuel qualified for sale under the 2007 Energy Independence and Security Act, the intended audience might still be military purchasing agents, the functional unit might still be a MJ of fuel, and water stress might be the impact of interest. Further, whereas the system boundaries would remain the same, specifying the use of the impact method described by Pfister (2009) defines and identifies the types of water uses, the mechanisms to which water is returned to the environment, and their relationship to regional water stress to be accounted and assessed in the LCA.

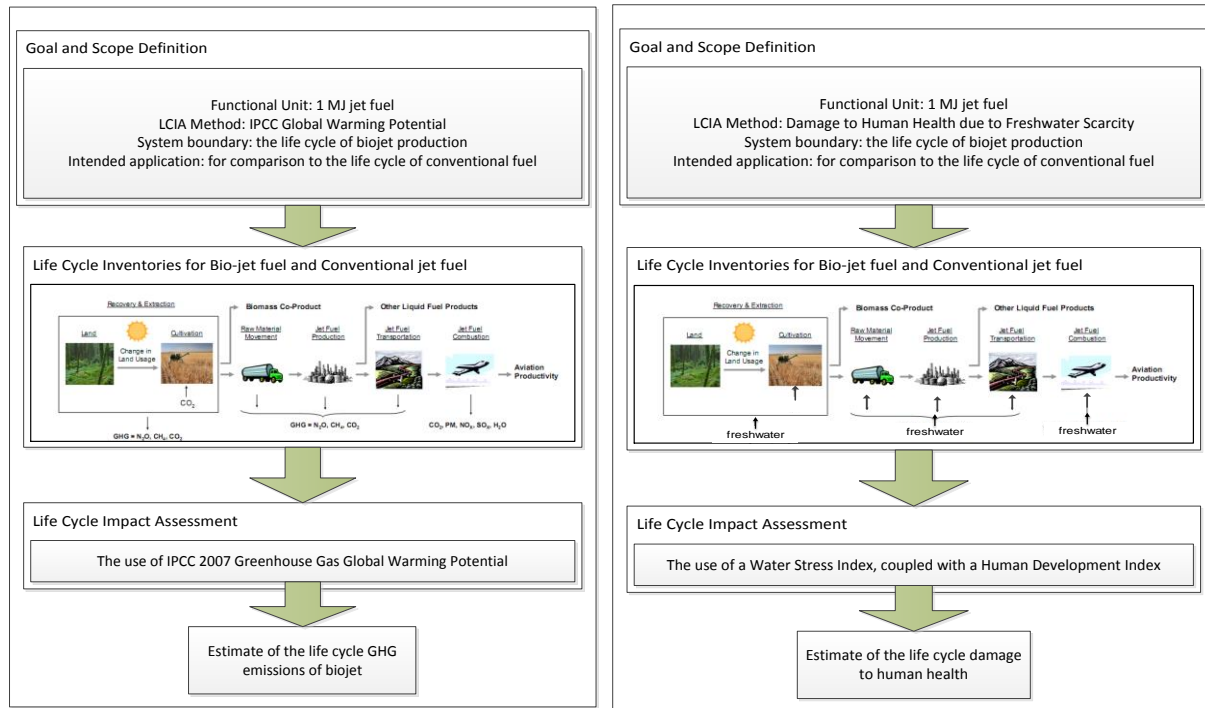


Figure 1: Example LCA procedural flow for bio vs. conventional jet fuel, with LCIA for greenhouse gas emissions (left), and damages to human health due to loss of water access (right).

1.2 Life Cycle Inventory Analysis

Following GSD is the LCI phase of LCA, during which resource use and waste are accounted for all life cycle processes in the system boundary. As described by Heijungs and Suh (Heijungs and Suh 2002), flows to and from the environment (e.g., extracted crude oil or freshwater from the environment and carbon dioxide emissions to the air and pesticide runoff to surface waters) are accounted for all processes within the system boundaries. Ideally, a complete LCI closes the mass balance such that all materials and energy into the product system are accounted for in what leaves the system.

Consider again Figure 1, where the LCA is intended to compare a biofuel and a conventional petroleum-based fuel. During the preparation of the LCI, materials and energy use and waste are accounted for all processes required for the production of each fuel. For the biofuel, the accounting process might use estimates of the amount of irrigation water, fertilizer, and pesticide used from the United States Department of Agriculture (USDA) Agricultural

Resource Management Survey (ARMS) and emission factors provided by the IPCC⁵ for the production of the feedstock crop; estimates of the amounts of feedstock crop and other resources (e.g., hydrogen) consumed and related emission factors for fuel production from a fuel hydroprocessing model such as described by Kahn and Cooper (2013); as well as fuel consumption and emission factors based on engine specifications and emissions tests. Subsequently, data representing resource use and emissions e.g., for the life cycle of the production of hydrogen might be collected from an LCA database⁶ to complete the inventory.

Although the use of data from LCA databases can greatly ease the preparation of a LCI, such databases provide single data values for inventory flows, with details concerning how these values were generated often vaguely described in supporting documentation and without meta data representing data uncertainty. These issues in data quality create serious challenges in transparency, modifying data to fit local technical uniqueness, and interpreting the significance of results with respect to data uncertainty. In response, the University of Washington Design for Environment Lab has been funded by the USDA National Agricultural Library to develop an LCI database for US field crops, the LCA Digital Commons (National Agricultural Library 2012), with inventory data represented as a set of parametric equations within each dataset as described by Cooper et al. (2012) and including measures of statistical uncertainty and variability (J.S. Cooper, Kahn, and Ebel 2011).

1.3 Life Cycle Impact Assessment

During the LCIA phase of LCA, resource use and waste accounted for in the LCI are characterized to estimate the contribution to the impacts of interest. Such “characterization” uses characterization factors to quantify the amount of impact per unit of each inventory flow. A characterization factor incorporates the results of fate and transport modeling and measure of the expected contribution to a given impact into a single weighting factor. In Figure 1, the IPCC Global Warming Potentials (GWPs) are used to characterize the contribution of life cycle air emissions such as carbon dioxide and methane to the environment to climate change. Similarly, the water stress indices developed by Pfister are used to characterize the contribution of water withdrawals from the environment to water stress (Pfister, Koehler, and Hellweg 2009).

⁵ See http://www.ipcc-nggip.iges.or.jp/EFDB/find_ef_s1.php?root=

⁶ Example LCI databases are listed at <http://faculty.washington.edu/cooperjs/Research/database%20projects.htm>

Characterization factors can be categorized as midpoint and endpoint indicators. The European Commission-Joint Research Centre - Institute for Environment and Sustainability (Centre 2011) define a category endpoint as an attribute or aspect of natural environment, human health, or resources, identifying an environmental issue giving cause for concern (International Organization for Standardization. 2006). Hence, an endpoint model (or a damage approach) is a characterization model that provides indicators at the level of Areas of Protection (natural environment's ecosystems, human health, resource availability) or at a level close to the Areas of Protection level. Alternatively, a midpoint characterization model provides indicators between emissions/resource consumption and the endpoint level within the cause-effect chain. For example, for a category endpoint of reduction in human health due to malnutrition, a reduction in the availability of drinking water might be a midpoint indicator.

For the development of characterization factors, the ISO standards recommend a series of steps: identify the relevant impact category endpoints, define a category indicator for the relevant endpoints, and categorize the LCI results to the appropriate indicator (performed through a characterization model).

Contribution to climate change is perhaps the most widely recognized LCIA impact category, with the IPCC GWPs as the most often used characterization factors. Example endpoints for the contribution to climate change are global temperature change, sea level rise, or loss of species diversity. The category indicator for these endpoints chosen by the IPCC is radiative forcing or the difference between radiant energy received by the earth and energy radiated back to space (Change 2007). The GWPs thus use detailed fate and transport models to represent changes in atmospheric chemistry/radiative forcing associated with a variety of air emissions.

Continuing the fuels/climate change example in Figure 1, the final combustion of bio or conventional fuel releases carbon dioxide (CO_2), methane (CH_4), and nitrous oxide (N_2O) (among other constituents) to the atmosphere. The relevant GWPs are specific to each type of emission and are presented relative to CO_2 as CO_2 equivalents ($\text{kg CO}_2\text{e}$). For example, the IPCC 100-year GWP for CH_4 is 25 $\text{kg CO}_2\text{e}$ (Forster et al. 2007) which indicates that on a mass basis an emission of 1 kg of CH_4 contributes 25 times the radiative forcing of a kg of CO_2 .

Unlike the use of GWPs as an LCIA impact characterization factor, methods applied to other impacts including the water stress index developed by Pfister (2009) as depicted in Figure 1 and others described in Section 2.4.2 are regarded with less consensus with related methods still developing. Considering the impact of water use as an

example, category indicators range from total water abstracted (Sauer et al. 1994), to evaporative use of irrigation water (Wu et al. 2009), to the estimation of a “water footprint” that attempts to capture all direct and indirect evaporate uses of water (A.Y. Hoekstra and Hung 2002).

Within this context, in their review of outstanding issues with LCA, Reap et al. (Reap et al. 2008) identify several challenges surrounding adequate impact assessments. For existing impact assessment methods⁷, issues identified include an incomplete or poorly defined set of category indicators and characterization models, poor or no representation of spatial variation and local environmental uniqueness, and inappropriate time horizons. Current LCIA methods in general neglect consideration of spatial variation in characterization of final disposition of emissions and the associated risk to humans and ecosystems, as well as varying levels of persistence due to local climactic, topographic, demographic, or hydrographic conditions. Or, when these are considered, the methods have been limitedly applied and are sometimes misused (e.g., models representing European conditions are used in other regions). Although not an issue for global impacts such as climate change, accurate and reliable impact assessment requires varying levels of specificity depending on the scope of the impact, when impacts are local or regional, regionally specific characterization factors are required for impacts such as depletion of freshwater resources.

The ISO standards recommend using existing LCIA methods when they exist, provided they adequately meet the needs of the study. For those needs that are not met, new methods for impact assessment must be developed.

Related indicators should be physically relevant and characterization models should be described by an environmental mechanism, be transparent, and be reproducible. Also, for LCAs to be used in comparative assertions, sensitivity and uncertainty analysis *must be performed*.

1.4 Interpretation

Finally, an LCA is completed during the interpretation phase, including the use of sensitivity, uncertainty, and data quality analyses to make and critique study results. The interpretation phase addresses issues in implementation of the inventory and impact phases. Robustness and representativeness of the model is explored through a sensitivity analysis, and uncertainty is propagated from the inventory data to the results, as well as a characterization of the effects of data quality on the results of the study. Results and recommendations are generated through contribution

⁷ See as examples:

<http://www.usetox.org/>

<http://www.epa.gov/nrmrl/std/sab/traci/>

analysis and comparison to alternatives and alternative scenarios. Recommendations can include changes or adoptions within the product studies, or further refinement of the model.

For example, during the interpretation phase and again referring to Figure 1, it may be found that a majority of combustion emissions of CO₂ from a biofuel are offset by the uptake of CO₂ during plant growth or that the majority of water use occurs during field crop irrigation. A contribution analysis for various modeled scenarios can also identify where the greatest weight of water use is over the life cycle, and the role of irrigation in the total water inventory. Also, a sensitivity analysis can use a Monte Carlo simulation to reveal which water use parameters have the largest impact on the variability of the life cycle results.

Persistent issues associated with the interpretation phase of LCA include: consistent representation and propagation of uncertainty, and a transparent and comparable method for the reporting of data quality. Current LCI data and impact characterization models/factors either do not include any basic statistical uncertainty information (e.g. sampling error), or provide only an “expert opinion-based estimate of uncertainty that can be expected as a result of low data quality” (e.g., a mismatch in the location or timeframe of the data as compared to the system of interest) (Frischknecht et al. 2005). Uncertainty estimates based on data quality can be arbitrary, are difficult to reproduce, and have been misinterpreted as representing statistical uncertainty. A true statistical representation of data uncertainty is critical to reliable LCA, since in many cases the range of confidence intervals can be many times the estimates themselves (J.S. Cooper, Kahn, and Ebel 2011). From this work, Figure 2 presents as an example the range of relative standard error (RSE) in crop production data developed for the LCA Digital Commons. Although the vast majority of the data have a RSE less than 100%, values range from zero to 1,600%.

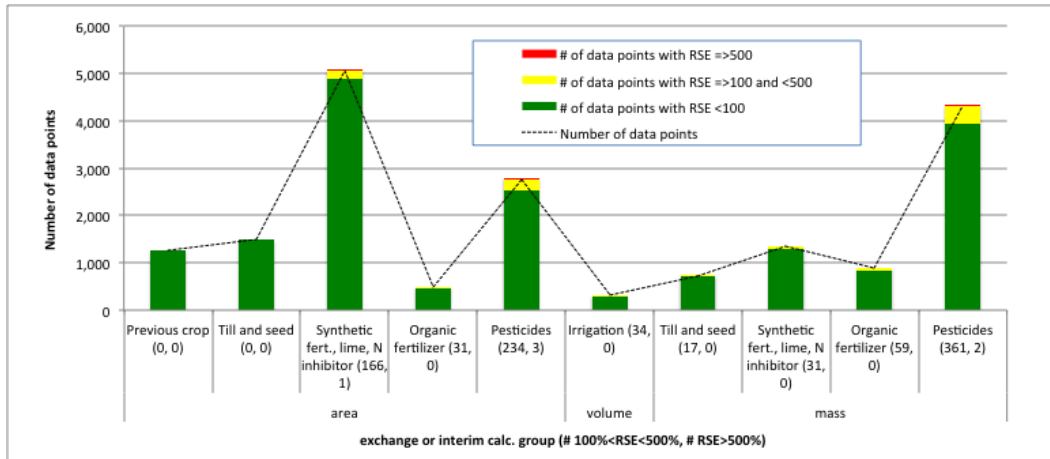


Figure 2: Exchange and interim calculation data by variable group and units of measure

Due to the data intensive nature of LCA, a practitioner often cannot avoid using data with varying levels of quality and uncertainty information. Thus, in the interest of transparency as well as for standards compliance, LCAs are required to address data quality for time-related coverage, geographic coverage, technology coverage, precision, completeness, representativeness, consistency, reproducibility, sources of the data, and uncertainty of the information (International Organization for Standardization, 2006). Commonly applied data quality analysis methods use a set of pedigree scores, ranging from 0 - 5 or 1 - 5, with the lower numbers corresponding to higher data quality in each of the ISO data quality categories (Figure 3). Cooper and Kahn (Joyce Smith Cooper and Kahn 2012) identify issues of subjectivity in commonly used scoring systems, making them not repeatable. They propose a more consistent and robust data quality analysis method that presents data quality thresholds such that for each data point, the practitioner reports whether it meets or does not meet a given threshold (Table 1).

Table 3 – Pedigree matrix for managing cost data quality issues in eco-efficiency					
Indicator score	1	2	3	4	5
Reliability of source	Verified data based on measurements	Verified data partly based on assumptions or non-verified data based on measurements	Non-verified data partly based on assumptions.	Qualified estimate (e.g. by industrial expert)	Non-qualified estimate or unknown origin
Completeness	Representative data from a sufficient sample of sites over an adequate period to even out normal fluctuations	Representative data from a smaller number of sites but for adequate periods	Representative data from an adequate number of sites but from shorter periods	Representative data but from a smaller number of sites and shorter periods or incomplete data from an adequate number of sites and periods	Representativeness unknown or incomplete data from a smaller number of sites and/or from shorter periods
Temporal differences	Less than 0.5 years of difference to year of study	Less than 2 years difference	Less than 4 years difference	Less than 8 years difference	Age of data unknown or more than 8 years of difference
Geographical differences	Data from area under study, same currency	Average data from larger area in which the area under study is included, same currency	Data from area with slightly similar cost conditions, same currency, or with similar cost conditions, and similar currency	Data from area with slightly similar cost conditions, different currency	Data from unknown area or area with very different cost conditions
Further technological differences	Data from enterprises, processes, and materials under study	Data from processes and materials under study from different enterprises, similar accounting systems	Data from processes and materials under study but from different technology, and/or different accounting systems	Data on related processes or materials but same technology	Data on related processes or materials but different technology

Figure 3: Data quality pedigree matrix. From (Ciroth 2009) and (Weidema and Wesnaes 1996)

Uncertainty and variability refer to the range of possible or expected values or outcomes. In the context of LCA, this range of expected outcomes would be the range of values of the life cycle impact for the production of the functional unit defined in the study Goal and Scope. Herein, the distinction is made between variability and uncertainty. Variability is the range of values that exist due to variations in the system being modeled. An example of variability in inventory assessment could be the range in emissions profiles associated with crude oil producing nations. An importer sourcing crude oil from around the world would be responsible for a range of environmental impacts. Uncertainty is the range of values that exist due to gaps in knowledge of the system being modeled. Returning to the example of the oil importer, uncertainty can exist in the environmental profiles of the exporting nation, due to incomplete monitoring of oil extraction activities.

Uncertainty and variability information for product flows and impact assessment methods is notably absent from most LCA databases, with the exception of the ecoinvent⁸ database. Ecoinvent uses expert opinions to determine

⁸ See <http://www.ecoinvent.ch/>

the level of uncertainty associated with a data quality score for each of the data quality categories. Thus a quantitative estimate of uncertainty is developed for each point in the database, based on a subjective and qualitative assessment of data quality. In the ecoinvent database, uncertainty is represented as a logarithmic distribution, with the magnitude of uncertainty reported as the geometric standard deviation. However, the expert opinion is based upon the data quality score, without consideration of the associated flow. Thus, a wide range of flows from across the technosphere and environment share the same uncertainty value, which is clearly unphysical and illustrative of the amount of uncertainty not considered in ecoinvent's uncertainty estimation..

Table 1: LCA Digital Commons flow data quality scoring criteria (Joyce Smith Cooper and Kahn 2012)

Category	Requirements for a data quality score of A
1. Reliability and reproducibility	The flow data were based on measurements using a specified and standardized measurement method OR The flow data were estimated using methods and data described in specified archival or other consistently publically available sources.
2. Flow data completeness	The flow data were collected over at least 3 years for agricultural (crop, livestock, forest, range) processes or other processes in which the data point varies for uncontrolled annual conditions (e.g., weather) AND The flow data balance the mass and energy in and out of the unit process. ⁹
3. Temporal coverage	The flow data represent operations that occurred between the unit process start and end dates without forecasting.
4. Geographical coverage	The flow data represent operations that occurred within the location of the unit process, including non-agricultural process data that have been adapted to reflect logistics and market shares ¹⁰ for the unit process location.
5. Technological coverage	The flow data represent the process(es) and/or material(s) specified without surrogacy or aggregation with other technologies.
6. Uncertainty	The flow data either include estimates of the first quartile, mean, median, and third quartile values OR data or probability distribution from which these values can be estimated.
7. Precision	The relative standard error of the flow data is less than or equal to 25% OR The interquartile range divided by the median is less than or equal to 50% OR For a triangular distribution, the minimum flow data value is $\geq 75\%$ and maximum flow data value is $\leq 125\%$ of the most likely value OR For a uniform distribution, the minimum flow data value is $\geq 75\%$ and maximum flow data value is $\leq 125\%$ of the average of the minimum and maximum values.

2 Research Goals, Motivation, and Broader Impacts

The approach taken by the LCA community for the development of LCIA methods for freshwater consumption has been theoretical, defining a methodology to map water use inventories to common LCA endpoints. Operationalized

⁹ An incomplete mass balance may represent either an incomplete unit process or an incomplete set of emissions factors, or both. In the case of a score of B for an incomplete set of emissions factors, the data quality analysis serves to highlight an opportunity to improve data quality through methodological or documentation improvement.

¹⁰ Market shares, sometimes called mixer processes in LCA, reflect the technologies used in local markets. For example, market shares are used to represent the mix of technologies used in regional electricity generation (the percentage of coal, natural gas, nuclear, etc. per kWh) and the mix of waste management technologies (landfilling, waste-to-energy, etc.) locally available.

LCA techniques seek to produce answers at a level of aggregation high enough to make comparisons across different technological alternatives. In order to make substantive “comparative assertions”, impacts must be aggregated and normalized to a sufficient degree so alternatives can be compared at a reasonable level of parity. To achieve this level of comparability, LCA practitioners have developed a set of indicators general enough to capture a wide range of environmental interventions, so alternatives that may have vastly different environmental flows, or locally realized environmental impacts, can still be compared, contrasted, and developed.

At present, inventory results are aggregated to end-point indicators with no representation of complexity of the coupling between the techno-environmental systems. Using the example of freshwater consumption, what is relatively simple to model at the small scale (the evapotranspiration of water at the farm level), is highly complex to scale up to the larger global spatial resolution that LCA attempts to represent. Examples of complex interactions include:

- Changes in precipitation due to the atmospheric recycling of applied irrigation water, changes in evapotranspiration due to land cover, and subsequent recharge of freshwater sources.
- Changes in irrigation requirements due to runoff from other irrigation water users.
- Characterization of impacts of freshwater consumption due to total availability, ie: how stressed are a region’s water resources, and what is the current ecosystem response.

This work demonstrates the importance of uncertainty and variability characterization in Life Cycle Assessment, using the study of a crop production unit process as an example. Each step of the LCIA procedure introduces some amount of uncertainty with the implementation of each characterization model, as well as natural variability associated with the variable nature of nature. For LCA to be used in comparative assertions between alternatives, the amount of variability and uncertainty in the results must be characterized. Below, a detailed examination of uncertainty and variability in the estimation of green and blue water consumption is presented.

2.1 Characterization of Water Consumption in LCA

Water is a critical element, playing a vital role across a range of scales, from providing a vital life supporting role at the microscopic level, to being one of the key ingredients to ecosystem function and climactic cycling. It has always been a critical part of industrial civilization, playing a wide set of roles through the technosphere. Water is used in

resource extraction, power generation, industrial cooling, industrial washing, as a solvent, it is used for recreation, for irrigation, and for transportation. Two critical distinctions separate water from other abiotic resources inventoried in LCA (such as bauxite or crude oil): many freshwater sources are renewable, often on a yearly basis (thus a certain amount of water can be sustainably withdrawn), and water may be used many times without being consumed.

Water exists in the environment in many locations, but freshwater is available for human uses in only a few. Supply is generally defined as either from surface or groundwater sources. Surface water sources include free flowing rivers, and natural lakes, or regulated streams and reservoirs. Groundwater can be a layer of water in the soil matrix, recharged by precipitation, and coupled to nearby surface water bodies through lateral soil moisture, or groundwater can be geologically separated from surface water bodies and not subject to annual recharge or any recharge at all. Groundwater sources without recharge are known as fossil groundwater sources, as they represent ancient water deposits not coupled to the surface water cycles.

2.2 Terms and Definitions

Three classes of parameters are associated with freshwater use; the source of the water, the fate of the water, and whether it was applied as a part of an anthropogenic activity or is naturally occurring soil moisture. Terms and definitions for water use in LCIA are based upon the foundational work by Owens (Owens 2001) who made key distinctions in fate and sources of freshwater. The primary distinction in fate is between the **consumption** of and the **use** of freshwater. Freshwater **use** refers to any water that has provided some type of service either in – stream or off – stream (such as following a withdrawal). Examples of off-stream freshwater use—productive use following a withdrawal or abstraction of a water resource—include thermoelectric or industrial cooling, in municipal water supplies, or irrigation. In-stream freshwater use is water used in situ such as for boating and recreation, maintaining fisheries, or for in-stream hydroelectric generation. Freshwater **consumption** is water that has been used, and is no longer available in its originating basin. Examples of water consumption are evaporative losses from irrigation or cooling, or embodiment within a product. The importance of the distinction between used and consumed water is the contribution of the activity to a change in the availability of a water resource. Consumed water is no longer available to other users in the originating watershed, while un-consumed water that has been used is still available to

other users. Thus, for impacts associated with freshwater availability and resource depletion, it is the quantity of water consumed, and its type of origin, that is important as an LCIA category indicator.

Owens also highlights the importance of the water source in estimating the impacts of freshwater consumption—particularly, whether consumed water originates as either surface or groundwater. Surface and groundwater sources may recharge at varying rates. Surface water sources, such as lakes, rivers, and reservoirs, often recharge at a seasonal time-step and can be managed to provide a consistent water resource. Depending on the local geology, groundwater aquifers may recharge along the same timescales as surface water sources, or may be geologically isolated from the surface water, and are thus non-renewable.

Hoekstra and Hung (A.Y. Hoekstra and Hung 2002) introduce freshwater consumption classification by water type as either green, blue, or grey water. Green water is a naturally occurring water resource that is not abstracted before its consumption, such as soil moisture due to humidity or precipitation. Blue water is water that has been withdrawn from its source and applied elsewhere and is further classified by the source of the blue water; either from surface or groundwater sources. Grey water is a quantity of freshwater necessary to dilute an emission to acceptable levels. Thus, it represents a functional loss of water, not an evaporative loss.

In summary, the following terms and definitions are used in the assessment of freshwater impacts:

- Water use – water that has provided some type of service.
- Water consumption – water that has been used and is no longer available in its originating basin.
- Green water – consumed water that originated as naturally occurring soil moisture, such as rainfall.
- Blue water – water that was withdrawn from a source (either surface or groundwater) and consumed off-stream.
- Grey water – the amount of freshwater necessary to dilute an emission to acceptable levels.

2.3 Literature review: assessment of water consumption in LCA

In 1994, Sauer et al. (1994) used LCA to compare disposable and cotton diapers. They found no clear homerun winner between the two diaper options – whereas there is a reduction in solid waste by replacing disposal diapers with cotton diapers, the cotton diapers *use* additional water and energy associated with cotton production and diaper washing. Sauer et al. make the straight comparison between water used for pulp production with water used for

cotton production, diaper washing, and for irrigation (Figure 4). No consideration is made for the location of the water withdrawals, and the final disposition of the water used. Whereas most of the water used for the life cycle of disposable diapers is found to be in the pulp production phase, most of the water consumption for cotton diapers is found to be used for cotton growth and washing. Because cotton growth, pulp production, and laundry, all have a vast difference in water sources, points of withdrawal, and final dispositions, Sauer et al.'s work is now seen as misleading in its aggregation of various uses of water into a single water use inventory for comparison between alternatives.

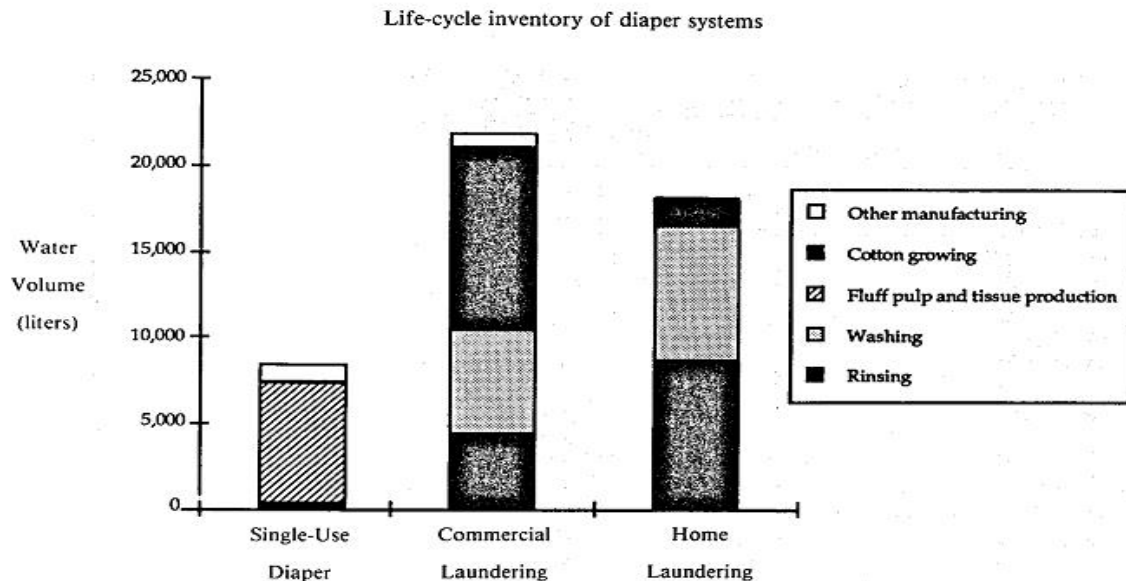


Fig. 3. Total water requirements for children's diaper systems, 1990.

Figure 4: Water use for diapers, from (Sauer et al. 1994)

Improving upon the work of Sauer et al., the 2001 work by Owens laid the framework for treating water impacts as a unique suite of impact categories instead of as a simple tracking of the inventory flow as an abiotic resource (described above). Owens made several propositions for what he called a "battery of indicators ... necessary to address different aspects of water resources in order to obtain a more complete and balanced perspective". The importance of the distinction between consumptive use (water withdrawn from a source is not available after use in its originating basin) and non-consumptive use (water either returned to the point of withdrawal or is used in-stream) is explained. Also, Owens requires that the source of water, either surface or groundwater, be reported to allow for

consideration of varying recharge rates and mechanisms of those sources, which are often location specific. For example, the fraction of a precipitation event that contributes to a river's baseflow, as opposed to percolating to groundwater or rapidly leaving the basin as floodwater, is dependent on local topology, soil structure, vegetation, and storm intensity, among other factors. Thus, identifying the source of withdrawal became a critical piece of information in determining the sustainable rate of use of that freshwater resource.

In addition to the concepts of Owens (2001) is the characterization of green or blue water (GW or BW respectively) as introduced in the context of the Virtual Water (VW) footprint (A.Y. Hoekstra and Hung 2002). VW refers to all water consumed during the production of a product or service; with green water representing a naturally occurring resource such as soil moisture from local precipitation, and blue water including all water diverted from its origin such as ground or surface water applied to a field of crops.

Based on the work of Owens (2001) and leveraging the concepts of VW footprints, several frameworks for LCIA of freshwater have been proposed. Rolf Frischknecht et al. (2005) present a set of eco-factors based on a water stress index (a dimensionless number representing the impact of water withdrawal) linking freshwater consumption to ecological scarcity, and Stewart and Weidema (2005) propose representing freshwater impacts as energy required to produce an alternative water source. Pfister et al. (2009) provide the next in-depth work and define category endpoints as damages to human health, ecosystem quality, and resources, and use a suite of characterization models to map them to freshwater consumption. Damages to human health is characterized through a water stress index and through a human development index, the assertion being the more developed the nation, the better equipped it is to handle stress to freshwater resources. Damage to ecosystem services is characterized by a reduction in net primary production, and damage to resources is estimated by rates of freshwater withdrawal relative to recharge. That is, if withdrawal exceeds recharge, the water source is being depleted. Work related to that of Pfister et al includes that of Mila i Canals et al. (2008) who scale resource depletion by units of antimony, a metal used to normalize depletion of various resources to a common equivalence, in the same vein as scaling greenhouse gas emissions to CO₂ eq. Van Zelm et al. (2011) use net primary production to estimate loss of species diversity from groundwater extraction in the Netherlands. Bayart et al. (2010) propose a framework to estimate freshwater consumption associated with the loss of water function due to emissions of pollutants, ie: grey water consumption, a framework further developed by Boulay et al. (2011). Thus, three classes of freshwater impacts methods can be defined:

- Volumetric approaches, such as the virtual water footprint. These approaches are simply the aggregation of the green, blue, and grey water types.
- Impact-oriented approaches, such as those proposed by Pfister et al. and others. These approaches are an extension of volumetric approaches, in that they further characterize water consumption to other mid or end point impacts.
- Distance-to-target type approaches, such as those proposed by (Stewart and Weidema 2005) which characterize water use impacts by impact associated with generating the next best available technology.

One point in common of methods in all three categories is the need to differentiate water consumption from water use. Thus, no matter the approach employed for LCIA or for water footprinting, the estimation of freshwater consumption is the first step to characterizing water use impacts. The following section reviews approaches used in literature for estimation of green, blue, and grey water consumption.

2.4 Estimation of green and blue water consumption in literature

Green water consumption (GW) is an estimate of the amount of naturally occurring soil moisture that is consumed due to the production of a product. In the case of agricultural production, GW is estimated as the amount of effective precipitation (P_{eff})¹¹ that is lost due to the evapotranspiration of a growing plant (ET). The ET of a crop is the combined value of the evaporation from the soil and the transpiration of water through the plant and is considered the theoretical maximum amount of water that can be consumed. Any effective precipitation in excess of a crop's ET cannot be consumed by the production of that crop, thus does not contribute to water scarcity—it either stays in the soil, or leaves the field as either surface runoff or deep percolation. Thus, GW can be estimated as the minimum of either the P_{eff} or the ET – that is, if the effective precipitation is greater than the evapotranspiration, then the total green water consumed is equal to ET, otherwise, there is less precipitation than potential to consume it, and so green water consumed is equal to P_{eff} .

Blue water consumed (BW) is that amount of applied water that is consumed by ET. Assuming irrigation water is applied in response to a shortage of soil moisture, the maximum amount of BW possible is the difference between the GW and ET, known here as the crop water deficit. Thus, if GW is equal to ET, there is no more potential for

¹¹ P_{eff} : defined in the National Engineering Handbook (NRCS 1993) as the part of rainfall that can be used to meet the needs of growing crops, not including surface runoff or percolation below the crop root zone

evapotranspiration and no applied water is consumed. If GW is less than ET, the effective precipitation is below the potential for water consumption, and so BW can be equal to that amount up to the difference between GW and ET (this algorithm is explored further in section 3.1.3). That is, for blue water consumption, if water is applied uniformly and at a rate below the rate of soil water saturation, the amount of blue water consumed will equal the amount of water applied, up to the potential ET or the maximum amount of ET that would occur if excess water is in the ecosystem. In summary, the following additional terms and definitions are used to estimate green and blue water consumption:

- Evapotranspiration (ET). The combination of water evaporated from the soil, and transpired through the plant stomata during crop growth.
- Effective precipitation (P_{eff}). The amount of total precipitation that is available to crops via soil moisture, accounting for evaporation during rainfall, percolation due to water exceeding soil capacity, and runoff due to precipitation rate exceeding soil infiltration rates.
- Crop water deficit (CWD). The crop water deficit is the difference between the maximum ET of healthy, well watered plants and the effective precipitation. Thus, it is the amount of water plants need that is not being met by rainfall.

Various models have been applied in previous studies to estimate green and blue water consumption. Mishra and Yeh (2011) use the CROPWAT (Swennenhuis et al.) model to estimate GW, and the 2008 Farm and Ranch Irrigation Survey (FRIS) for BW (NASS 2008). Peters et al. (Peters et al. 2010) apply a similar approach in the context of Australian red meat production. Some who have implemented the CROPWAT model have also modeled P_{eff} using the Soil Conservation Service (SCS) method (NRCS 1993) ((Milà i Canals et al. 2008), (Chapagain and Orr 2009), (Mishra and Yeh 2011)). For the estimation of ET, Chapagain and Hoekstra (2004a) use FAO's CROPWAT model (Swennenhuis et al.). This work is an implementation of the FAO56 method and is based on the Penman-Monteith equation that captures evaporation from radiation and momentum transfer, and is the recommended approach by FAO for estimating crop water needs at the farm level (Allen et al. 1998). Other studies use variations of the FAO56 method, adapted to conditions specific to Australia (Peters et al. 2010) or California (Fingerman et al. 2010). Fingerman et al. (2010) estimate ET as described by Orang et al. (Orang, Snyder, and Matyac 2005) in an FAO56-based assessment of crop production in California counties and considers the resulting

ET estimate to be the total water consumed. Other applications of the FAO56 method include the work of Mila i Canals et al. (2008) who study the case of broccoli grown in Spain, and base their freshwater consumption inventory on the adaptation of FAO56 described by Chapagain and Orr (2009) in their study of Spanish tomatoes.

For water application, some studies either assume it is equal to the Crop Water Deficit (CWD) (the difference between ET and P_{eff}) or simply use a national average ((Pimentel and Patzek 2005) and (King and Webber 2008)). Other researchers use farm survey data, such as the Farm and Ranch Irrigation Survey (FRIS) or the Agricultural Resource Management Survey (ARMS) in the U.S.. Although uncertainty information accompanies the FRIS and ARMS data, it has not been included in any of the studies reviewed. Interestingly, data representing a single year from the FRIS were used in four studies found in the literature to estimate blue water consumption only (Chiu, Walseth, and Suh 2009), (Scown, Horvath, and McKone 2011), (Wu et al. 2009), (Harto, Meyers, and Williams 2010). **Herein, we note concern with the use of a single year of data, clearly centered around precipitation, climate, irrigation, and other annual variations.**

For uncertainty in the water applied, many of the above studies note the spatial variation in depths of water application and percentage of the area to which water is applied, and have treated variability in U.S. irrigated agriculture as the spatial variation of the range of estimates calculated for major crop producing states ((Chiu, Walseth, and Suh 2009), (Dominguez-Faus et al. 2009), (Scown, Horvath, and McKone 2011), (Mishra and Yeh 2011)). However none of these works consider variability and uncertainty in other data, such as uncertainty in collected applications data (i.e., sampling error) and uncertainty in and applicability of local environmental data driving crop growth and ET. Also, water consumption as a result of manure application has not been considered.

In estimating water consumption, several studies among previous works base both green and blue water consumption directly on the Water Footprint of Nations database, an implementation of the VW concept (Chapagain and Hoekstra 2004a). Water consumption is calculated assuming GW is any VW originating as soil moisture and BW is the Crop Water Deficit (CWD). Studies that use the results directly from the Water Footprint of Nations to estimate total crop water consumption in a LCA related study include Pfister, Koehler, and Hellweg (Pfister, Koehler, and Hellweg 2009), Dominguez-Faus et al. (Dominguez-Faus et al. 2009), and van Breugel et al. (Van Breugel et al. 2010). However, the Water Footprint of Nations gives no indication of the sources of blue water, and

these studies assume that the crops are not in a condition of water stress and that farmers apply sufficient irrigation water to satisfy the crop water balance.

2.5 Estimation of grey water consumption in the literature

Although not treated specifically in this dissertation, a review of current approaches for grey water consumption is presented. For grey water the intent is to represent degradation in water quality or functionality as a result of waterborne pollution and grey water consumption (GrW) has been differently defined by different researchers. In the water footprinting effort by UNESCO IHE and as implemented by the Water Footprint Network, GrW is defined by Hoekstra and Hung (2002) as the amount of freshwater required to dilute a pollutant to a minimum freshwater quality standard. Thus, Hoekstra and Hung 's GrW is not the physical consumption of water, but instead represents the loss of freshwater function, or depletion of water due to a reduction in quality. Because the many users of freshwater have varying quality requirements, GrW is based upon the range of user requirements (e.g., drinking, steam production, or as cooling water).

More recently, Bayart et al. (2010) reviewed various approaches to characterizing grey water consumption, including applying the distance-to-target and functional approaches. The distance-to-target is based upon the LCIA method of Stewart and Weidema (2005) that uses the amount of energy required to improve water quality to a minimum standard as a normalizing approach to grey water consumption. For example, in a region without adequate water treatment, the distance-to-target approach may underestimate consumptive impacts due to lack of available water purification technology. Also in 2010 and in their study of Australian red meat production, Peters et al. (2010) make note of the various changes in freshwater quality due to non-consumptive freshwater use, using qualitative categories, such as high, medium, and low, but they do not offer a recommendation as to how to treat changes in quality.

In 2011, Boulay et al. (Boulay et al. 2011) describe water impacts as a loss of function, therefore supporting the scope of water impacts through the use of functional analysis. They generate a “functionality based, regionalized inventory method allowing impact assessment associated with quality degradation and consumption.” The functional approach quantifies the amount of grey water consumed by measuring the total amount of freshwater required to dilute a pollutant to its maximum concentrations. Specifically, Boulay et al. identify 11 categories of water users with distinct water quality requirements: 3 types of domestic users, industrial users, once-through

cooling, 2 types of irrigation, freshwater aquaculture, hydropower, transport, and recreation, as listed in Table 2. The authors use thresholds from the World Health Organization (WHO) and the United Nations Environmental Programs (UNEP) for agriculture, FAO for fisheries, WHO and the European Economic Community for drinking water, WHO and the Quebec government for recreation, the Electric Power Research Institute for cooling water and the Taiwan EPA for “several users”. Each user group is defined by a minimum freshwater quality standard (see Table 3: Boulay et al. (2011) example water quality thresholds), and the typical freshwater processing available to improve water quality before use. The list of parameters, and their thresholds provided by Boulay et al. provide an extensive point of reference for grey water consumption indicators. Based upon the varying needs of the identified water users, Boulay et al. also define a set of water quality classifications, and the associated uses that can be accommodated by those classes (Table 4). It also provides a baseline for comparison with other water quality standards, such as that of the USEPA, or those prescribed at the state level (Environmental Protection Commission 2011).

Table 2: Freshwater user groups. Boulay et al. (2011)

Table 1 Types of water users

Water user	Definition
Domestic 1	Domestic user performing no treatment or simple chemical disinfection to the water prior to use
Domestic 2	Domestic user performing a conventional chemical–physical treatment (coagulation or precipitation, solid removal process, disinfection) or equivalent treatment to the water prior to use
Domestic 3	Domestic user performing an advanced treatment (i.e. conventional treatment plus additional treatment (UV disinfection, adsorption, etc.)) or specific advanced treatment (reverse osmosis, nanofiltration, adsorption, ion exchange, desalination, etc.) or desalination to the water prior to use
Industrial	Industrial user (manufacturer) withdrawing available water and treating it to the required level
Cooling	Once-through cooling water for energy production
Agriculture 1	Agriculture that requires good quality irrigation water
Agriculture 2	Agriculture that requires only poor-quality irrigation water
Fisheries	Freshwater aquaculture and capture of fish
Hydropower	Hydroelectricity production
Transport	Transportation of goods through inland waters
Recreation	Recreational activities such as swimming and water sports

Table 3: Boulay et al. (2011) example water quality thresholds¹²

Parameter/element	Symbol	Units	Agriculture 1	Agriculture 2	Fisheries	Domestic 1
Chloramines	NHnCl(3-n), where n = 0, 1 or 2	mg/l			0.1 (temporary threshold since no threshold is provided in FAO93)	3 (Drinking water standard of WHO08)
Chlorine dioxide	ClO2	mg/l			0.1 (temporary threshold since no threshold is provided in FAO93)	5 (Drinking water standard of WHO08)
Aluminium	Al	mg/l	5 (WHO06: problematic in acid soils only)	5 (FAO85 & WHO06: problematic in acid soils only)	0.05 (FAO93)	
Ammonia	NH ₃	mgN/l			0.3 (TAI98; FAO93 mentions much lower values for salmonids)	0.05 (EEC75)
Antimony	Sb					0.02 (Drinking water standard of WHO08)
Arsenic	As (mg/l)	mg/l	0.1 (WHO06: wide toxicity range from 0.05 to 12)	0.1 (WHO06: wide toxicity range from 0.05 to 12)	3 (FAO93; lower limit of the toxicity range)	0.01 (Drinking water standard of WHO08)
Barium	Ba	mg/l				0.7 (Drinking water standard of WHO08)
Beryllium	Be	mg/l	0.1 (WHO06: wide toxicity range from 0.5 to 5)	0.1 (WHO06: wide toxicity range from 0.5 to 5)		
Bicarbonate	HCO ₃ ⁻	mg/l	500 (WHO06)	500 (WHO06)		
Boron	B	mg/l	3 (WHO06)	3 (WHO06)		0.5 (Drinking water standard of WHO08)
Cadmium	Cd	mg/l	0.03 (WHO06: conservative limit due to its potential for accumulation)	0.03 (WHO06: conservative limit due to its potential for accumulation)	Absence (FAO93 toxicity range from 0.0002 to 0.001)	0.003 (Drinking water standard of WHO08)
CaSO4		(mg/l) ²				
Chloride	Cl ⁻	mg/l	350 (WHO06: severe effect for surface irrigation)	350 (WHO06: severe effect for surface irrigation)		250 (aesthetic recommendation, WHO08)
Chromium (total)	Cr total	mg/l	0.1 (WHO06: conservative value due to lack of information)	0.1 (WHO06: conservative value due to lack of information)	Absence (no clear threshold in FAO93)	0.05 (Drinking water standard of WHO08)
Copper	Cu	mg/l	0.2 (WHO06: wide toxicity range from 0.1 to 1)	0.2 (WHO06: wide toxicity range from 0.1 to 1)	0.05 (temporary value = average value of FAO93's range for maximum copper concentration)	2.0 (Drinking water standard of WHO08)
Cyanide	CN-HCN	mg/l			Absence (FAO93's range for maximum cyanide concentration is from 0.002 to 0.02)	0.07 (Drinking water standard of WHO08)

¹² Table taken from the supporting information of (Boulay et al. 2011)

Boulay et al. recommend applying grey water consumption to LCIA as a change in basin wide functionality based upon a set of water category functional groups defined by the quality thresholds identified (see Table 4). Ambient or current water category functionalities have been estimated by the authors for many global watersheds. To determine if the water functionality has changed classes requires a system wide assessment of total pollutant flows into the water shed of interest. Although this approach benefits from being based on a physical and measurable mechanism, it does not conform with ISO LCA model structure, a change in basin wide functionality is not an indicator that can be applied to a functional unit, as defined in the goal and scope definition, unless the functional unit represents the entire product system. Thus, many of the goals of performing LCAs such as identification of process improvement or of environmental burden of alternatives is not feasible at the scales required to use this method.

Table 4: Freshwater quality functionalities. Boulay et al. (2011)

Quality	1	2a	2b	2c	2d	3	4	5	Rain
Sources	S or G	S or G	S or G	S or G	S or G	S or G	S or G	S or G	Rain
Quality level	Excellent	Good	Average	Average-Toxic	Average-Biologic	Poor	Very poor	Un-usable	
Contamination	Low microbial low toxic	low microbial medium toxic	Medium microbial medium toxic	Low microbial high toxic	High microbial low toxic	High microbial medium toxic	High microbial high toxic	Other	N/A
Domestic 1	√	X	X	X	X	X	X	X	√
Domestic 2	√	√	√	X	X	X	X	X	√
Domestic 3	√	√	√	√	√	√	√	X	√
Agriculture 1	√	√	X	√	X	X	X	X	√
Agriculture 2	√	√	√	√	√	√	X	X	√
Fisheries	√	X	X	X	√	X	X	X	√
Industry	√	√	√	X	X	X	X	X	√
Cooling	√	√	√	√	√	√	√	X	√
Recreation	√	√	X	√	X	X	X	X	√
Transport	√	√	√	√	√	√	√	√	√
Hydro	√	√	√	√	√	√	√	√	√

√ functional, X non-functional

In an alternative measure of grey water effects, Liu et al. (2012) define their grey water footprint not as a volume of water consumed, but instead as an indicator of a nutrient load's "appropriated assimilation capacity" due to specific pollutant discharges into a water body by using the naturally occurring concentration of the pollutant in the receiving water body as a characterization factor. The result is then aggregated with the footprints of other pollutants into a total water footprint:

Equation 1: Grey water footprint of Liu et al. 2012

$$GWF = \sum_i \sum_j \left(L_{add\ i,j} / C_{max\ i,j} - C_{net\ i,j} \right)$$

where $L_{add\ i}$ is the addition of pollutant i to a water body, $C_{max\ i,j}$ is the maximum allowable concentration of pollutant i in body j , and $C_{net\ i,j}$ is the ambient concentration of pollutant i in body j . Liu et al. calculate ambient or natural nutrient loads at unpopulated rivers, and then apply the basic values to a set of river basin archetypes by assessing 300 watersheds for natural nutrient loads, comparing them to values of background nutrients of other watersheds from the literature. These background loads are used to normalize bulk emissions by assimilation capacity to generate the footprint.

2.6 Research needs for the estimation of green, blue, and grey water consumption

Although there is, as of yet, no agreement on how best to model freshwater use impacts in LCA, all of the myriad approaches outlined above identify freshwater consumption as an appropriate category indicator. Despite these efforts, however, there is still a need for a set of freshwater consumption indicators that meet the data quality needs as outlined in Owens (Owens 2001) and Table 1. The water footprinting work by Hoekstra and Mekonnen (Arjen Y Hoekstra and Mekonnen 2012) is perhaps the most complete attempt at a set of volumetric water consumption indicators, representing green, blue, and grey water consumption. Their green water consumption estimation is based upon the soil moisture model available at the ISRIC World Soil information database¹³ and report a water footprint for various industrial sectors at a 5' (arc-minute) resolution. However, Hoekstra and Mekonnen assume that blue water consumption is equal to the crop water deficit without consideration of the quantity of irrigation water applied, which often leads to overestimation of water consumption. In addition, their grey water consumption is based upon the work of Liu et al (Liu et al. 2012) (described below), which estimates a loss of assimilative capacity based upon 300 watershed archetypes, an estimate that is not readily compatible with green or blue water consumption indicators. In addition, the authors present an entire water footprint inventory at a 5' resolution, equal to their most resolved dataset. It can be argued that the precision of an estimate is dependent on the least resolved parameter, not the most.

Of those studies that estimate green water consumption, many do so using the CROPWAT model. CROPWAT is distributed with a climate dataset, CLIMWAT, which provides all of the required climate parameters, at a low resolution, roughly a dozen for the continental United States. In addition to the low spatial resolution, CLIMWAT also has no representation of uncertainty or temporal variability (see Mishra and Yeh (2011) (Milà i Canals et al.

¹³ <http://www.isric.org/>

2008), (Chapagain and Orr 2009), (Mishra and Yeh 2011)). The CROPWAT model (Swennenhuis et al.) is an implementation of the FAO56 method (Allen et al. 1998, 56), a sophisticated climate based estimation for crop specific ET that requires data for local temperature, relative humidity, and wind speed. Whereas temperature is a fairly common climate measurement, long term measurements of relative humidity and wind speed are available at only a handful of locations in the United States. Although state averages are reported for these studies, the estimates are based on only several locations within each state, and do not necessarily capture climate heterogeneity (see Figure 5). Two of the studies reviewed use an implementation of FAO56 refined to either Australia (Peters et al. 2010) or California (Fingerman et al. 2010), but neither include temporal variation in green water consumption, reporting instead only climate averages. **Thus there exists a need for a better understanding of the impacts of data availability and climate fluctuations on the certainty of green water consumption estimates.**

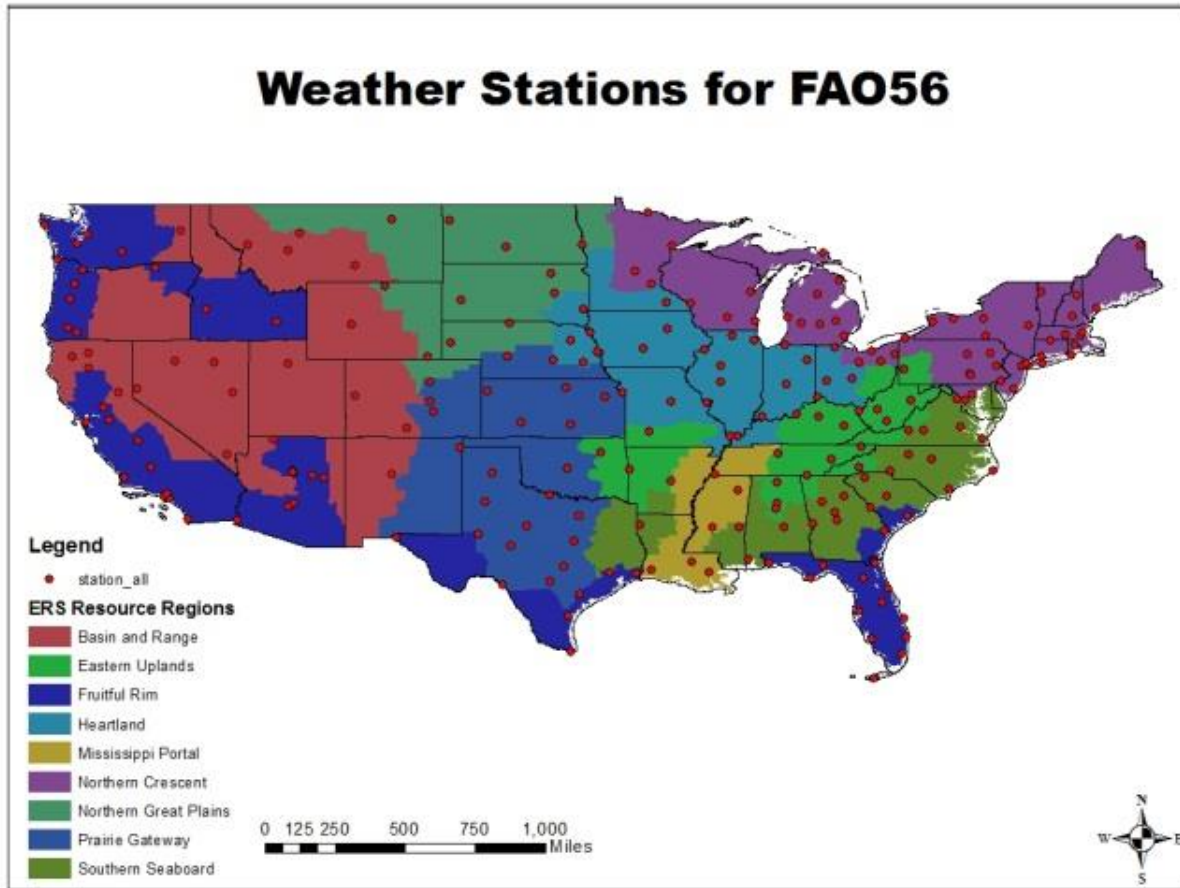


Figure 5: Weather stations with data for FAO56 method¹⁴

2.7 Description and research needs of impact-oriented approaches.

In review of the current work for the new ISO water footprint standard (“ISO/DIS 14046 - Environmental Management -- Water Footprint -- Principles, Requirements and Guidelines” 2013), Berger and Finkbeiner survey several outstanding methodological challenges, for which uncertainty and variability play a critical role (Berger and Finkbeiner 2012). Product water footprint methods are classified into one of two classes: volumetric and impact-oriented approaches. A volumetric water footprint estimates the total water consumption from the three freshwater compartments: green, blue, and grey water (the work of (Arjen Y Hoekstra and Mekonnen 2012) being an example of a volumetric approach). The volumetric methods produce a quantification of water consumed, for a product, and do not attempt to perform further characterization. Because they treat green, blue, and grey water consumption on

¹⁴ <http://www.ncdc.noaa.gov/oa/climate/climatedata.html#surface>

equal footing by aggregating them together, volumetric approaches are not appropriate for making comparative assertions. For example, a unit of green water is not equal to a unit of blue water, since this would imply that if the crop production were to not take place, the green water would not be consumed. This does not consider that other land uses also have a green water consumption profile, ranging from parking lot (all runoff, and no consumption), to forests (high consumption). However, impact-oriented methods have their own challenges, which are discussed in greater detail below.

Impact based methods attempt to map water consumption to generalized end-point indicators, such as those defined by the eco-indicator 99 method (Goedkoop and Spriensma 2001). Several impact based approaches have been identified in the literature (see previous sections), and share a common approach to characterization modeling.

Both volumetric and impact-oriented approaches begin with the quantification of freshwater consumed as described in previous sections of this dissertation. For volumetric approaches, the characterization modeling ends at the estimation of freshwater consumption. For impact-oriented approaches, the next step in the characterization modeling is to characterize freshwater consumption in terms of the level of regional water stress. This is done with the application of water stress indices, based upon some form of a utilization-to-availability ratio which can be applied as a type of characterization factor; the lower the water stress index, the lower the impact of the water consumption. Some authors (e.g.: Pfister, Koehler, and Hellweg 2009) map water stress adjusted consumption to established endpoints such as human health, ecosystem quality, or resource damages, that can be aggregated with endpoint impacts from other environmental flows such as toxins, greenhouse gases, or raw materials.

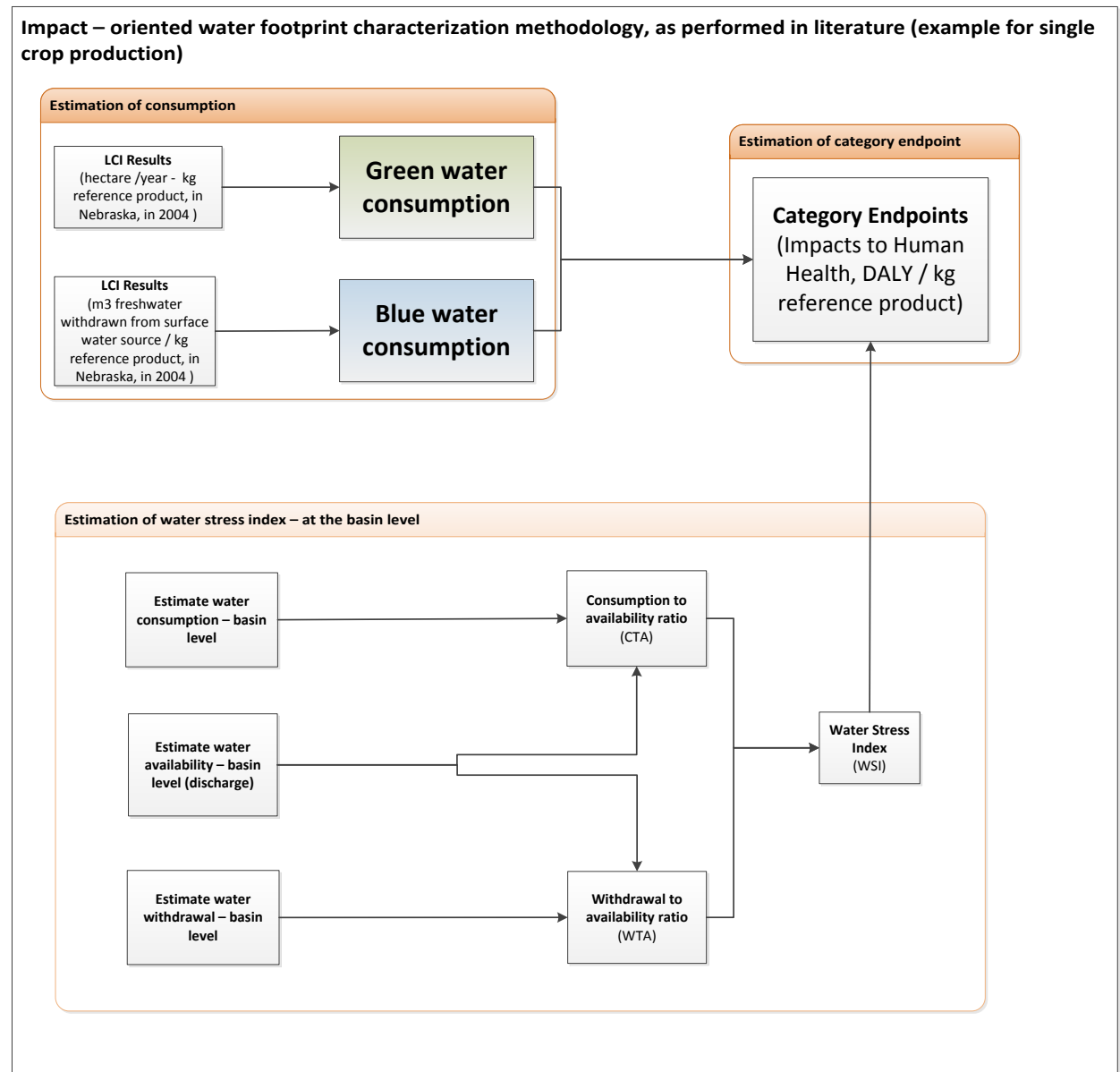


Figure 6: Typical characterization modeling scheme for water footprints, example Impacts to Human Health

The characterization modeling scheme typical for water footprinting (for example (A. Hoekstra et al. 2011)), and water characterization in LCIA (for example (Pfister, Koehler, and Hellweg 2009)) follows the general outline in Figure 6. In this diagram, environmental impacts are mapped for land use and water application flows from the LCI results to an example category endpoint. Three pathways are represented: estimation of a water stress index at top, followed by green water and blue water characterization below. The level of impact of water consumption is dependent upon the level of water stress within a basin. Thus, category endpoints are regionalized by water stress indices, which scale the quantity of water consumption by the level of demand for that resource.

Water stress indices are based upon the amount of water use within a basin relative to the amount of water available—known as either a Withdrawal-to-Availability ratio (WTA), or a Consumption-to-Availability ratio (CTA). To calculate WTA, the total amount of water withdrawn from a basin is estimated for all users and industries, over a timescale of interest. Water availability is estimated as all renewable resources within a catchment over the same timescale. An estimate of CTA is calculated in a similar fashion—the total amount of water consumed within a basin is estimated for all users and industries, over the timescale of interest.

As an example, to facilitate water sustainability studies as part of a water footprint analysis, Hoekstra et al. model WTA (Equation 2) (A. Hoekstra et al. 2011) as the sum of domestic, industrial, and agricultural withdrawals (D , I , and A respectively), divided by the difference of the total catchment discharge and the environmental water requirement (Q and E respectively).

Equation 2: Water withdrawal to availability ratio, as used by (J. Hoekstra et al. 2010)

$$WTA = \frac{\sum D+I+A}{\sum Q-E}$$

A Water Stress Index is derived from estimates of WTA or CTA by a number of approaches. The following examples are from the review paper of Brown and Matlock, who indicate three general classes of water stress indices (Brown and Matlock 2011b):

- Indices based upon meeting basic human water requirements: such the Falkenmark indicator, per capita use versus regional availability (Equation 3)
- Human water requirements, including non-domestic uses such as industrial and agricultural production (Equation 4)
- Indices including environmental and ecological water requirements (Equation 5).

Equation 3: Falkenmark indicator, m³ water use per capita

$$WSI = \frac{m^3 used}{capita}$$

Equation 4: WSI, as the sum of domestic, industrial, and agricultural uses (D, I, and A respectively), divided by the sum of all discharges (Q)

$$WSI = \frac{\sum D + I + A}{\sum Q}$$

Equation 5: WSI as the average of hydrological, environmental, life, and policy indicators (H, E, L, and P respectively)

$$WSI = \frac{H + E + L + P}{4}$$

The common goal of all of these classes of approaches is to identify a level of sustainable water withdrawal for a particular region. These indices have been integrated into LCIA methodologies as a means to characterize the level of intensity of water use on a particular region: one unit of consumption in a high stress region will have a greater impact than the same unit of consumption in a low stress region. Thus, water stress indices are employed as a second characterization model, scaling the impact of water consumption by the level of economic, ecological, and human dependence on the water resource. The water consumption indicator, adjusted by the WSI, can be considered a secondary mid-point category indicator, and is known as a level of water deprivation or contribution to water deprivation at certain thresholds. For the volumetric approach of Hoekstra et al., the intensity of water consumption is determined as follows:

- $WSI > 1$; **Overexploited stress.** Water withdrawal is exceeding maximum sustainable uses and some ecological demands are not being met.
- $0.6 \leq WSI \leq 1$; **Heavily exploited.**
- $0.3 \leq WSI < 0.6$; **Moderately exploited.**
- $0 \leq WSI < 0.3$; **Slightly exploited**

In the case of overexploitation, the withdrawals are exceeding the total discharge available for anthropogenic uses, thus presumably water that is required for ecological services, and/or water from non-renewable deposits are being used.

Impact-oriented methods tend to take a more sophisticated approach to developing WSI. For example, the authors Pfister et al. use a measure of WSI to estimate the impacts of water consumption on human health. They compensate for the variation in precipitation's contribution to increased water stress, as well as the impacts of strongly regulated flows (SRF), by adjusting WTA with a variation factor (Equation 6) (Pfister, Koehler, and Hellweg 2009). The variation factor (VF) used to adjust the WTA is derived from the standard deviation of monthly and yearly precipitation data from 1961 to 1990 (Equation 7 where s_{mth} and s_{yr} are the monthly and annual standard deviation, respectively). Water stress is then modeled as a logistic function, ranging from 0.1 to 1, tuned for the threshold between moderate and severe stress = 0.5 (corresponding to WTA = 0.4) (Equation 8).

Equation 6: Water-to-Availability ratio adjusted by variation factor (VF) (Pfister, Koehler, and Hellweg 2009).

$$WTA^* = \begin{cases} \sqrt{VF} \times WTA & \text{for SRF} \\ VF \times WTA & \text{for non - SRF} \end{cases} \quad (-)$$

Equation 7: Variation factor for the adjustment of WTA (Pfister, Koehler, and Hellweg 2009).

$$VF = e^{\sqrt{\ln(s_{mth})^2 + \ln(s_{yr})^2}} \quad (-)$$

Equation 8: WSI as a logistic function of withdrawal-to-availability (WTA)

$$WSI = \frac{1}{1 + e^{-6.4 \cdot WTA \cdot \left(\frac{1}{0.01} - 1\right)}} \quad (-)$$

To estimate a final category indicator, WSI is used as a characterization factor for water consumption. To model the impacts on damage to human health, Pfister et al. combine the physical water stress index with impact factors derived from estimates of basic human need and exposure to depletion in water resources (Equation 9). The estimate of WSI is multiplied by the percent of total regional water *use* for agricultural production ($\% WU_{ag}$), which is multiplied by the ratio of Human Development Factor (*HDF*- unitless) to Water Requirement to avoid malnutrition ($m^3/yr\text{-capita}$). The final impact category is scaled by a Damage Factor (*DF*) in units of Disability Adjusted Life Year (DALY) per m^3 of freshwater consumed, which characterizes the loss of life in terms of time due to malnutrition.

Equation 9: Estimate of damage to human health due to malnutrition as a result of freshwater consumption (Pfister, Koehler, and Hellweg 2009)

$$\Delta HH_{malnutrition} = [WSI * \%WU_{ag} * \frac{HDF}{WR * DF}] * WU_{consumed} \text{ (DALY/m}^3\text{)}$$

2.8 Criticisms and research needs for scaling impact-based approaches

In their progress review of standard development for ISO 14046, Berger and Finkbeiner outline several critiques and research needs for both volumetric and impact-oriented approaches. Critiques focus on the applicability of either approach to system analysis, and the challenges of interpretation in making comparisons between water footprints of products. Research needs include an improved representation of the impacts of spatial scale, and characterization models with a more transparent connection to the physical impact mechanisms. Overarching all of these research needs is a representation of uncertainty, which is recognized as a critical component to decision making and is required for LCAs to be used in comparative assertions (International Organization for Standardization 2006).

Scaling water consumption from the farm scale to the basin scale is a major gap in current impact-oriented approaches. At any scale, some portion of precipitation originates from beyond the control volume, the balance having originated from within control volume. This phenomenon is known as atmospheric recycling, and is conceptually modeled as the mass balance of water within a vertical column over some area. The atmospheric water balance used for recycling models is presented as Equation 10, where w is the atmospheric moisture storage, \bar{v} is the horizontal wind velocity, and E and P are the local evapotranspiration and precipitation, respectively.

Equation 10: Atmospheric water balance

$$\frac{\delta f}{\delta t} + \nabla * f * \bar{v} = E - P \text{ (units of } L/T\text{)}$$

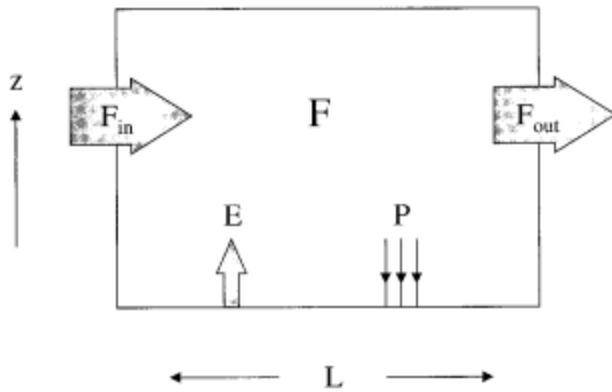


Figure 7: Schematic representation of 1-D atmospheric water balance (Trenberth 1999), where F is the moisture flux, L is the length scale, and E and P are the same as they are in Equation 10.

In plain language, Equation 10 states the change in atmospheric moisture storage (the precipitable water vapor) is equal to the difference in evapotranspiration and precipitation, minus the horizontal water vapor flux (a simplified schematic is presented in Figure 7, from (Trenberth 1999)). Thus, the atmospheric water balance is the vertical integration of the water vapor flux into and out of a region. Integrated over time, the total precipitation (P_t) in an area is equal to the precipitated moisture from local evapotranspiration (P_e), and the precipitated moisture from advection (P_a) (Equation 11). The amount of precipitation originating from within the basin is determined by solving the water mass balance.

Equation 11: Total precipitation as the sum of vapor from advection and evapotranspiration

$$P_t = P_a + P_e$$

Equation 12: Atmospheric recycling ratio: precipitation due to local ET over total precipitation

$$\rho = P_e / P_t$$

The recycling ratio (Equation 12) is dependent on the scale of the control volume. At the global scale, the recycling ratio is 1, since the advection component of the mass balance is zero. All precipitation originates from evapotranspiration from within the control volume. As the length scale of the control volume decreases, so does the recycling ratio. At the point scale, all precipitation originates from outside of the control volume. Basins or catchments define physically relevant control volumes—all precipitation occurring within a basin contributes to the water supply of that basin. Herein lays the importance of the basin as the system boundary originally defined by

(Owens 2001), the activities at the farm level impact the activities of other users within the basin. When considering the impact of water use, the impact of use at a farm must be considered at the basin scale. Thus, the level of atmospheric recycling at the scale of the system boundary must be considered: for basins with a positive recycling ratio, some water consumed at the farm level will reenter the water supply as recycled precipitation during the time frame of interest. That is, for basins with a positive recycling ratio, the water consumed at the farm level is greater than the water consumed that contributes to water scarcity.

In addition to local water consumption returning to its originating basin as recycled precipitation, water consumed can precipitate in adjacent basins. Two basins contributing flows to the life cycle of a single functional unit can be physically connected by this form of atmospheric moisture advection—water consumption in one location contributes to precipitation in another location. Recycled precipitation can feed crops directly as green water consumption, reducing the irrigation requirement, or can contribute to blue water supply, increasing the total water availability and reducing water stress. A revised characterization modeling scheme is presented in Figure 8, building upon the current approaches, but including atmospheric recycling.

The revised approach is similar to the flow diagram in Figure 6, however, there is the inclusion of atmospheric water recycling at the intersection of environmental flow characterization and WSI modeling. After the initial impact characterization (water consumption at the farm level), the fate of consumed water must be determined. Consumed water either: remains in the basin it was consumed in, precipitates over another basin within the product system, or leaves the product system (for example: as precipitation over the ocean, or to re-precipitate at a time beyond the temporal scope of the LCA).

Water remaining in the basin as precipitation contributes to water availability, reducing the impact of the water consumed to the total water stress of the basin, or can fall on crops, reducing the need of application of irrigation water. Similarly, water that enters a basin within the product system defined in the Goal and Scope section will also have a positive contribution to water scarcity. These credits must be incorporated into a final water footprint to fully realize the impact of the system under study. Finally, that water which leaves the product system all together is truly consumed by the definition of (Owens 2001) and others.

Impact – oriented water footprint characterization methodology, including atmospheric recycling (example for single crop production)

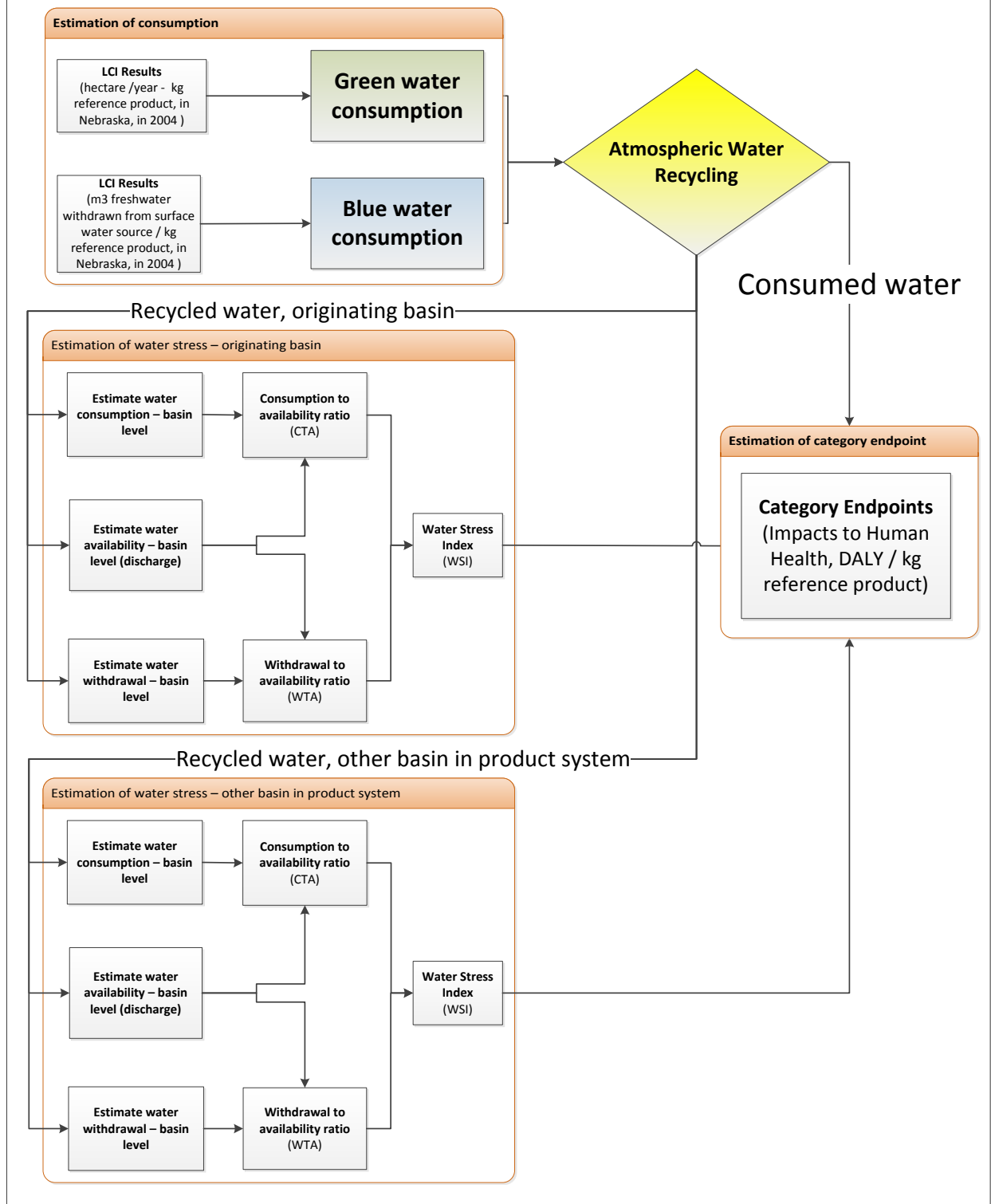


Figure 8: Characterization modeling scheme for water footprints, extended to include atmospheric recycling

2.9 Additional motivation for this Dissertation

This research is part of the development of the USDA LCA Digital Commons¹⁵ (National Agricultural Library 2012) database. The general goal of the Commons is to contribute to the field of LCA, through advancements in, and dissemination of, methods and data. To this end, the USDA Digital Commons is an *open source* on-line database and tool for use in LCA, hosted by the USDA for use in public and private sector decision making throughout the world.

The Commons data structure, designed by researchers in the University of Washington Design for Environmental Laboratory, is defined by four key features intended to support a wide range of bioproduct research. First, all of the key inventory data flows are represented as parametric equations within each data set, relating raw input data to inventory flows through a transparent set of mechanisms and models as described by Cooper, Noon, and Kahn (2012). In addition to allowing for transparency and verification, this formulation provides flexibility by allowing for the substitution of alternative raw data for individual flows or processes that may more accurately represent the system under study. This flexibility can become critical when performing comparisons between various scenarios, for exploring opportunities for impact reduction, or for material flow restructuring.

Secondly, the Commons data are accompanied by variability meta-data, as described by Cooper, Noon, and Kahn (2012) and Cooper, Kahn, and Ebel (2012). This provides several critical benefits: it allows for the estimation of the significance of differences in LCAs comparing alternative products and allows sensitivity analysis to be based on specific calculation parameters/raw data. Large amounts of variation, or a lack of statistical significance between alternatives in the study's results, may mean alternatives are not statistically different or may be an indication of an inappropriate study scope.

Thirdly, data quality is described as a set of thresholds for each data quality indicator, as noted in the preceding section and described in detail by Cooper and Kahn (2012); data either meets an explicitly defined quality threshold criteria, or it does not. Data quality thresholds allow practitioners to effectively describe the weaknesses in their studies, sources of potential uncertainty, and areas for further research in particular when suspect data are driving study results. Thus each raw data parameter in the LCA Digital Commons is accompanied by a seven term (each either A for pass, B for fail) data quality pedigree (J.S. Cooper and Kahn 2011).

¹⁵ See <http://www.lcacommons.gov/>

Finally, the LCA Digital Commons database is making a significant step forward in the design of its assessment framework by making a clear definition between the impact and inventory phases so that characterization models can be consistently and accurately applied. Although existing databases have been designed to work in concert with specific existing LCIA methodologies, some imbed fate and transport models (i.e., imbed the estimation of the movement through and degradation of contaminants in air, water, or soil) into the estimation of some inventory flows and others do not. For example, the ecoinvent database¹⁶ applies fate and transport to fertilizer applications but not pesticide applications in the inventory: estimating the nitrous oxide volatilizing to air from fertilizers but not the volatilization or degradation of pesticides. Further, for pesticides an alternative approach is taken in the development of data for the USDOE's Life Cycle Inventory Database¹⁷, where pesticide volatilization and degradation is modeled in the inventory data. If an LCIA model of pesticides considers pesticide volatilization and degradation and is used in a single LCA using data from both ecoinvent and the USDOE LCI database, whereas the ecoinvent inventory data would be compatible the USDOE data would not (the USDOE data would double count the volatilization and degradation). Instead, the LCA Digital Commons draws the boundary of the LCI around the constituents of all environmental flows, in the form that they are applied with no fate and transport considerations. Fate and transport is then consistently applied in the impact assessment phase. Efforts to be compatible with the various existing LCIA methods is assured in the Commons through a "cross-walk" or a converter that performs the necessary fate modeling in order to mesh with the LCIA method of interest.

This dissertation provides two additional LCA advancements for the LCA Digital Commons. First, it describes a repeatable method for the development of freshwater use and consumption data including statistical metadata for LCI. Second, it develops methods to characterize the impacts of freshwater consumption for LCIA, with statistical metadata.

The very general goal of this research is to contribute to the field of LCA, through advancements in methods and data, particularly in representation of uncertainty and variability. As noted above, substantial advances are needed in all phases in LCA. In the US as elsewhere, consideration of life cycle environmental impacts in public policy and consumer communication is driving demand for LCA. For example, the US 2007 Energy Independence and Security Act (EISA 2007) requires a comparison of fuel life cycle GHG emissions for governmental fuel purchasing

¹⁶ See <http://www.ecoinvent.ch/>

¹⁷ See <http://www.nrel.gov/lci/>

contracts. Also, Product Category Rules and Environmental Declarations (as in ISO 14025) use LCA for product comparison and market-driven improvement. These drivers are putting the reliability and representativeness of LCA under increasing scrutiny, making advances in data quality in particular critical for mainstream acceptance.

Among the broader impacts of this research is an improved understanding of data uncertainty and study scope for the freshwater consumption indicator in LCIA. The improved flexibility and transparency of the LCA Digital Commons data structure can facilitate integration of LCA into product development, allowing for multi-objective or pareto efficient design for environment (quantifying tradeoffs between design alternatives such as improvement to global warming potential vs. freshwater consumption). A better understanding of water consumption through a product life cycle can allow for identification of supply chain exposure to severe drought events, or improved siting of new facilities away from competing water users, impaired source or at risk ecosystems or populations. Within this context, the ISO is developing a standardized protocol for water LCIA, although a date of publication is not currently available (ISO - International Organization for Standardization 2012). It is intended for the results of this dissertation to contribute to the development of this standard and reinforce the importance of improved transparency, data quality representation, and geographic specificity of freshwater impacts in LCA.

In summary, the LCA Digital Commons project advances the field in six general areas, the latter two from this dissertation specifically:

1. Representation of inventory flow data as transparent parametric equations within data sets.
2. Representation of uncertainty and variability of the data.
3. Development of a transparent and repeatable method for the analysis of data quality.
4. Explicit and consistent use of rules for model use in LCA phases.
5. Representation of water use inventories for bioproduct LCAs.
6. Development of water consumption category indicators for the assessment of water scarcity.

2.10 Conclusions

It is concluded here that research need for agricultural LCAs for freshwater consumption impacts are the following:

1. **There exists a need for improved understanding of uncertainty in the estimation of green and blue water consumption at the farm level. In inventory analysis, this includes the role of fluctuations of**

water applications and associated data uncertainty. In impact assessment, this includes the role of model selection for the estimation of ET, and input data related to the precipitation available to the crop. Chapter 3 provides an in depth exploration of uncertainty in the estimation of green and blue water consumption.

2. **Given an understanding of farm-level uncertainties in freshwater consumption estimates, there exists a need for improved understanding of temporal and scaling effects in the estimation of green and blue water consumption at the regional level.** In impact assessment, this includes the role of data consistence and availability in estimates of atmospheric recycling of water. Chapter 4 provides an in depth exploration of temporal and scaling effects in the estimation of green and blue water consumption at the regional level.
3. **Given an improved understanding of farm and regional level uncertainties in the estimation of freshwater consumption impacts, there exists a need to explore alternative interpretations of the impact.** For example, exploration of the water-energy nexus promises to further support water related decision-making. Chapter 5 provides an example case study.

3 Assessing Water Consumption on-site

3.1 Impact characterization model

The model structure employed for this dissertation is adapted from the literature and has been designed to coincide with the data structure developed for the USDA LCA Digital Commons (Joyce Smith Cooper, Kahn, and Noon 2012), in which fate and transport is entirely in LCIA. Referring to Figure 9, the following steps are required to map a water use inventory flow to freshwater consumption. First, inventory analysis provides a quantification of water use/applications for a given crop yield. Next, in impact assessment freshwater consumption is estimated on the bases of environmental mechanisms such that effective precipitation and evapotranspiration govern green water consumption, crop water deficit and water applications characterize blue water consumption, and water quality thresholds characterize grey water consumption. Impacts can be mapped to midpoint or end-point indicators based upon the needs of the LCA practitioner. Finally, sensitivity analysis is used to identify parameters either requiring further data refinement, or to be included in the Monte Carlo estimation of uncertainty.

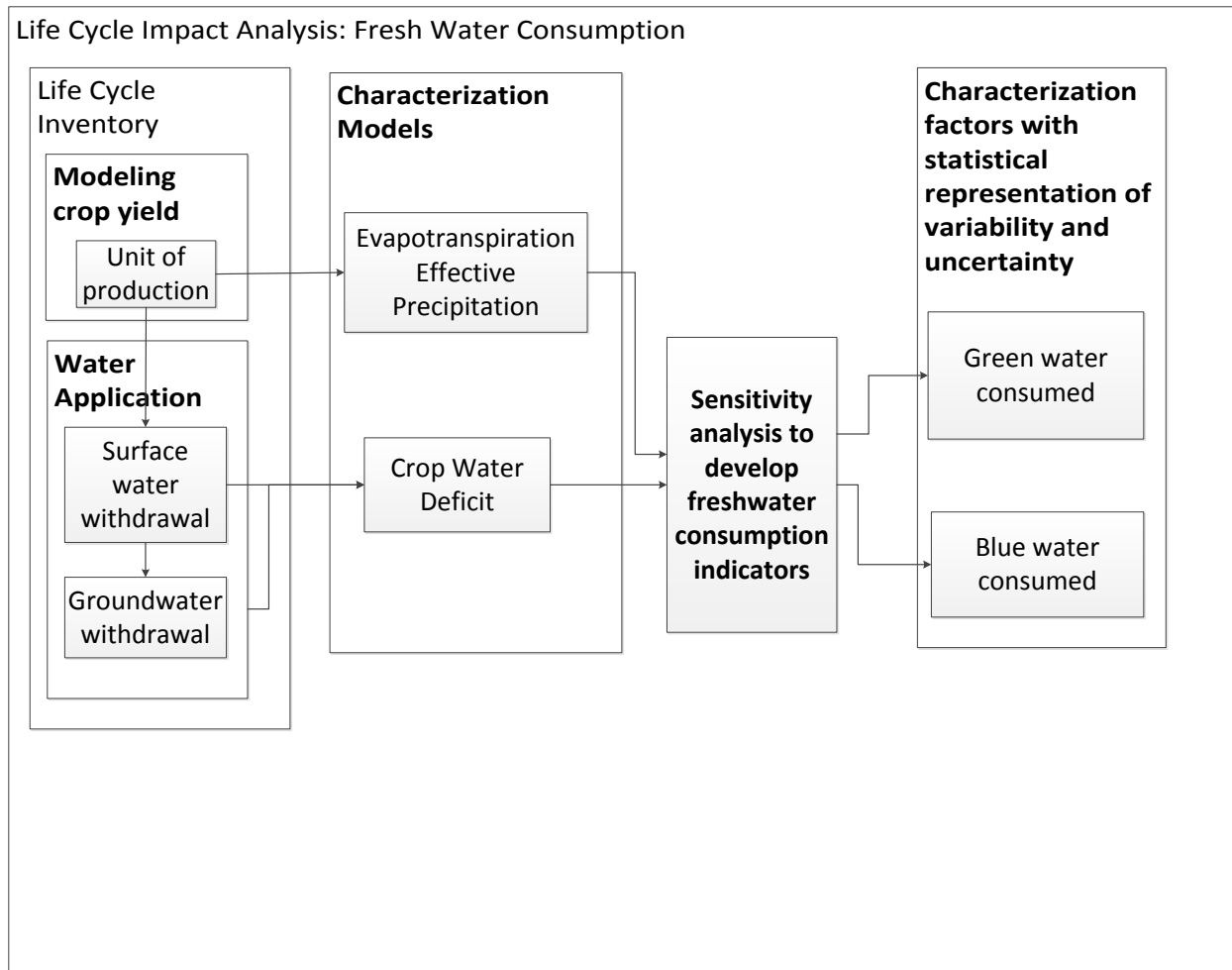


Figure 9: Model structure for freshwater consumption

Recall that freshwater consumption is defined as water that has been used, and is no longer available at its origin. In estimating characterization factors for field crop production, freshwater consumption is estimated by the hydrological water balance at the farm level (Figure 10) shown as Equation 13. For the farm as control volume, the total change in soil moisture is equal to the difference between incoming and outgoing water. Water enters the control volume as precipitation, capillary rise from groundwater, subsurface flow, and water applied as irrigation. Water leaves the control volume as surface run off, percolation through the soil, and subsurface flow. In Equation 13, F_{sub} is considered to be zero over large spatial scales for two reasons; either the ecosystem contains all of the originating water or the entering subsurface flows are balanced by the exiting subsurface flows. It is also common to consider the long time change in S_{moist} to be negligible, in consideration of the cyclical nature of seasonal climate. Capillary rise is also often neglected as crop root zone must be within a meter of the water table for it to

significantly contribute to available soil moisture (Allen et al. 1998). Thus, C_{rise} , F_{sub} , and S_{moist} are assumed to be de minimis and Equation 13 reduces to Equation 14. In the simplified water balance, green water consumption is that amount of P , the precipitation, which leaves the system by ET . Similarly, the blue water consumption is the amount of applied water, W_{app} , that leaves by ET .

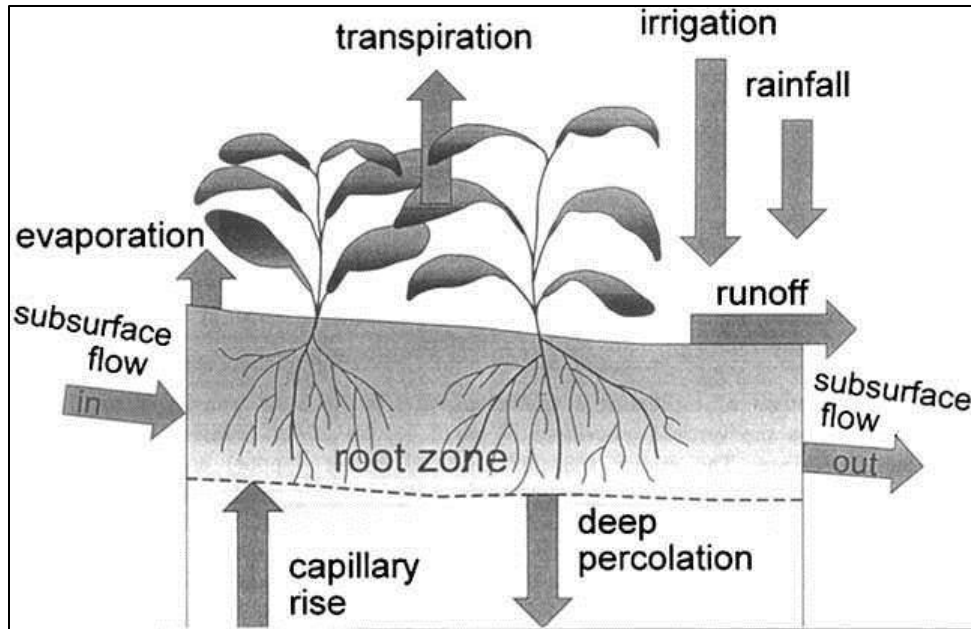


Figure 10: Water balance control volume, farm level¹⁸

Equation 13: Water balance at the farm level, (ET is evapotranspiration, W_{app} is water applied, P is precipitation, R_{off} is surface runoff, D_{perc} is deep percolation, C_{rise} is capillary rise, F_{sub} is subsurface flow, S_{moist} is total soil moisture)

$$ET = W_{app} + P - R_{off} - D_{perc} + C_{rise} +/ - \Delta F_{sub} +/ - \Delta S_{moist} \text{ (units of L)}$$

Equation 14: Simplified farm level water balance

$$(R_{off} + D_{perc}) = W_{app} + P - ET \text{ (units of L)}$$

Referring to Equation 14, if water is applied uniformly, and at a rate below the rate of soil water saturation (that is R_{off} and D_{perc} are zero), the amount of blue water consumed will equal the amount of water applied, up to the ET .

Assuming irrigation water is being applied due to a deficit in rainfall, green water consumed will equal the amount of precipitation at the field (up to an amount equal to ET). Thus, given estimates of the amount of water applied, the

¹⁸ Image from: (Allen et al. 1998)

LCA practitioner interested in quantifying freshwater resource impacts must estimate the ET, the precipitation available to the crop, and the associated uncertainty.

3.1.1 Modeling evapotranspiration

Potential crop ET (ET_c) is defined as the maximum amount of water that can enter the atmosphere by evaporation and transpiration through plant stomata (pore-like features in leaves). ET_c is a challenging value to determine directly, and there are a suite of approaches for developing ET_c estimates. ET_c can be estimated directly through standardized empirical approaches such as pan evaporation, indirectly by measuring flows in and out of a basin and solving the mass balance, or through various modeling approaches as is employed in previous LCAs. Here, three models have been employed, the FAO56 method (Allen et al. 1998), the Priestley – Taylor method (Dingman 2008), and the Hargreaves equation (Hargreaves and Allen 2003). These models implement what is known as the ‘ $kc - ET_o$ ’ approach; a two-step method where potential ET for a reference groundcover (ET_o) is first estimated based on local climate values, and then a crop specific coefficient (kc) is used to determine the value for ET_c at each time step. kc is an empirical parameter which scales ET_o to the characteristics of each crop (e.g., leaf area and growing rate) and the total ET_c is found by summing up all of the time steps at a specific location Equation 15.

Equation 15: The $kc - ET_o$ approach

$$ET_c = k_c ET_o$$

For this study, grass is used as the reference ground cover with the Penman-Monteith equation (Equation 16) used to estimate evaporation from radiation and momentum transfer.

Equation 16: FAO56 method, adaptation of the Penman-Monteith equation

$$ET_o = \frac{0.408\Delta(R_n - G) + \gamma \frac{900}{T + 273} u_2 (e_s - e_a)}{\Delta + \gamma(1 + 0.34u_2)} \text{ (units of } \frac{mm}{day} \text{)}$$

where Δ is the slope of the vapor pressure curve, R_n is the net incoming solar radiation, G is the soil heat flux density, γ is the psychrometric constant, T is the air temperature, u_2 is the wind speed at 2 meters above ground, e_s and e_a are the saturated and actual vapor pressures. This is the recommended approach by FAO for estimating crop water needs at the farm level (Allen et al. 1998), and is considered the baseline approach for this work.

As an alternative to the physical approach based upon the FAO56 method, the Hargreaves equation (Hargreaves and Allen 2003) provides an empirically developed regression for the Estimation of ET_o , requiring only maximum and minimum temperature and the latitude and elevation at the point of measurement:

Equation 17: The Hargreaves equation

$$ET_o = 0.0023(T_{ave} + 17.8)(T_{max} - T_{min})^{0.5} R_a \left(\frac{mm}{day} \right)$$

Where T_{ave} , T_{max} , and T_{min} are the average, maximum, and minimum daily temperatures respectively and R_a is the incoming extraterrestrial radiation. Although it does not benefit from the thoroughness of the FAO56 model, the simplicity of the Hargreaves method allows for more numerous estimates of reference ET as a result of greater data availability. Specifically, climate data for the application of the FAO56 and Hargreaves methods are available from the National Oceanic and Atmospheric Administration (NOAA) National Climatic Data Center¹ as 30-year climate normals for temperature and precipitation and as long time averages of relative humidity and wind speed. Figure 11 maps the locations of stations collecting data relevant to each method, at a total of 256 stations in the FAO56 method and 6,915 stations for solving the Hargreaves equation.

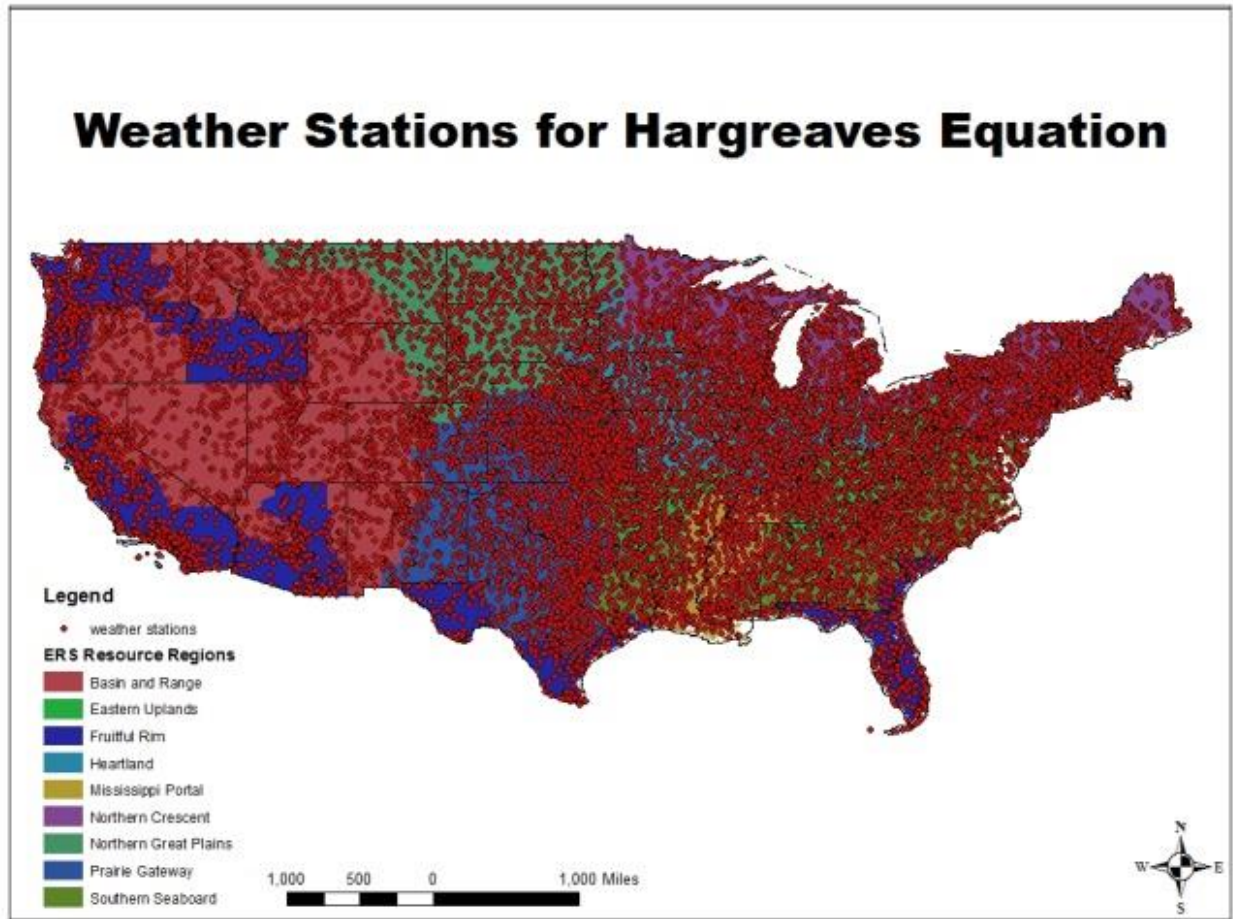


Figure 11: Weather stations with data for the Hargreaves equation

For use of all methods, at each time step the reference ET is multiplied by k_c which scales ET_o from reference grass to the crop of interest. k_c values are defined both for specific crops and for various points along the crop lifecycle: growth, mid (or mature), and end phases. General purpose k_c values are provided by Allen et al. (Allen et al. 1998) for use with FAO56 and were compiled by Chapagain and Hoekstra (Chapagain and Hoekstra 2004b) in the Water Footprint of Nations by general climate regions as listed for corn in Table 5.

Table 5: Corn crop coefficient data for $k_c - ET_0$ ¹⁹

	$k_{c\ ini}$	$k_{c\ mid}$	$k_{c\ end}$	L_{ini} (days)	L_{dev} (days)	L_{mid} (days)	L_{end} (days)	P_{date}
Tropics/Sub-tropics summer rain	0.3	1.2	0.5	20	35	40	30	15-Jun
Oceanic/Sub-tropics winter rain	0.3	1.2	0.5	30	40	50	30	15-Apr
Temperate/Boreal	0.3	1.2	0.5	30	40	50	30	15-May

Although Chapagain and Hoeskstra identify six general climate ecotypes, there are three different sets of k_c values: tropics/sub-tropics with summer rain, oceanic/sub-tropics with winter rain, temperate/boreal (the difference between the ecotypes being the planting dates and growth periods, not the coefficients themselves). The initial growth phase following the planting date is represented by $k_{c\ ini}$, a period when the plant is a seedling with a very small leaf area. The development phase (L_{dev}) is the period when the plant begins to produce significant leafy matter, the k_c value during this time is calculated by a linear interpolation between $k_{c\ ini}$ and $k_{c\ mid}$. The mature phase of the plant (L_{mid}) is when the leaf area is the greatest, and the potential ET is at a maximum. During the end phase (L_{end}), the plant becomes less productive, and its ET declines. The k_c value used during this period is a linear interpolation between $k_{c\ mid}$ and $k_{c\ end}$, the coefficient at time of harvest. The resulting time periods of k_c values for corn range from 125 to 150 days, and the planting dates range from mid-April to mid-June, as depicted in Figure 12.

¹⁹ * $k_{c\ ini}$, $k_{c\ mid}$, $k_{c\ end}$: initial, mid, end phase coefficients, respectively. L_{ini} , L_{dev} , L_{mid} , L_{end} : length of initial, development, mid, and end phases of corn lifecycle. P_{date} : planting date.

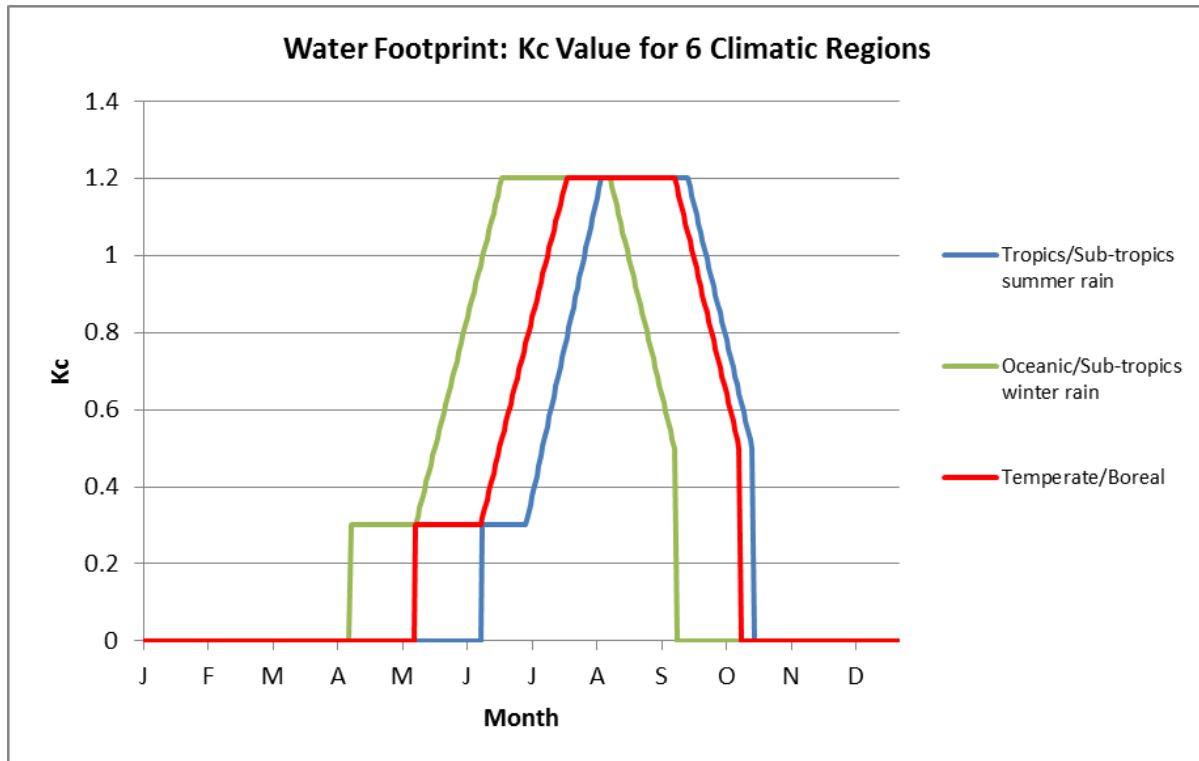


Figure 12: Crop coefficients from Chapagain and Hoekstra 2004

3.1.2 Modeling effective precipitation

During rain events, a fraction of actual precipitation stays in the control volume as soil moisture available to the plant. To estimate the amount of incoming precipitation staying as soil moisture, the SCS method is applied to estimate the *effective precipitation* (P_{eff}) (NRCS 1993). The estimation of monthly P_{eff} with the SCS method is defined as Equation 18 and Equation 19.

Equation 18: SCS method for effective precipitation

$$P_{eff} = SF(0.70917P_t^{0.82416} - 0.11556)(10^{0.02426*ET_c}) \left(\frac{in}{month}\right)$$

Where ET_c is the potential crop ET and SF is the soil saturation factor, dependent on D the depth of usable soil water storage, P_t is the actual monthly precipitation.

Equation 19: Soil saturation factor, SCS method for effective precipitation

$$SF = (0.531747 + 0.295164 * D - 0.057697 * D^2 + .003804 * D^3) (in)$$

The estimate of effective precipitation can exceed neither the total monthly precipitation, nor the local crop evapotranspiration. If the result of Equation 18 exceeds either, the value for effective precipitation is replaced with the lesser of those two values. Thus, the effective precipitation is further piece-wise defined as (Equation 20), and it follows that effective precipitation must be estimated after the estimation of ET_c .

Equation 20: Piece-wise definition of effective precipitation

$$P_{eff} = \min(P_{average}, ET_c)$$

3.1.3 Estimation of freshwater consumption

To estimate freshwater consumption, green and blue water data are collected and applied to Equation 21 and Equation 22 based on the work of Chapagain and Orr (Chapagain and Orr 2009). In both equations, an estimate is made at a monthly time step at individual weather stations and is based on the minimum of two governing parameters:

Equation 21: Green water consumption

$$GW_{cons} = \min(ET_c, P_{eff}) \left(\frac{mm}{month} \right)$$

Equation 22: Blue water consumption

$$BW_{cons} = \min(CWD, W_{app}) \left(\frac{mm}{month} \right)$$

Where ET_c is the potential crop ET, P_{eff} is the effective precipitation, CWD is the crop water deficit, and W_{app} is the quantity of water applied. The CWD (Equation 23) is the difference between the potential crop ET and the P_{eff} .

Thus, GW and BW are coupled through CWD (Equation 22) at each time step and at each location:

Equation 23: Crop water deficit

$$CWD = ET_c - P_{eff}$$

Equation 24: Crop water deficit

$$[\forall: CWD > 0, BW_{cons} > 0] \text{ and } [\forall: CWD \leq 0, BW_{cons} = 0]$$

Green water consumption is defined by Equation 21 as the minimum of either ET_c or P_{eff} . ET_c is the potential ET, and can be thought of as the upper limit of water the environment can consume. Thus, if P_{eff} is less than ET_c , there

is more potential for ET than there is moisture to consume, and GW is taken to equal P_{eff} . Conversely, if P_{eff} is in excess of ET_c , more moisture is present than can be consumed by the environment, thus GW is equal to the maximum possible ET, ET_c . Equation 22 is defined by the same reasoning, with BW as the minimum of the CWD and W_{app} . The CWD is the balance of P_{eff} and ET_c , if CWD is positive, there is potential for irrigation water applied to be consumed, but only up to an amount equal to CWD. W_{app} in excess of CWD cannot be consumed by ET, as the environment has exceeded its physical potential to do so. An assumption implicit in this approach is that water is only applied when a positive crop water deficit exists, and that the rate of application matches the soil saturation rate. Thus, runoff and percolation are assumed to occur only when water application exceeds crop water deficit; when $W_{\text{app}} > \text{CWD}$. After the estimation of GW and BW at monthly time steps and at each weather station location, total GW and BW is calculated by summation of all months in a year. The individual station results are then aggregated to the state level, to match the scope of the applied water data. The flow diagram of estimation of crop water deficit is displayed in Figure 13.

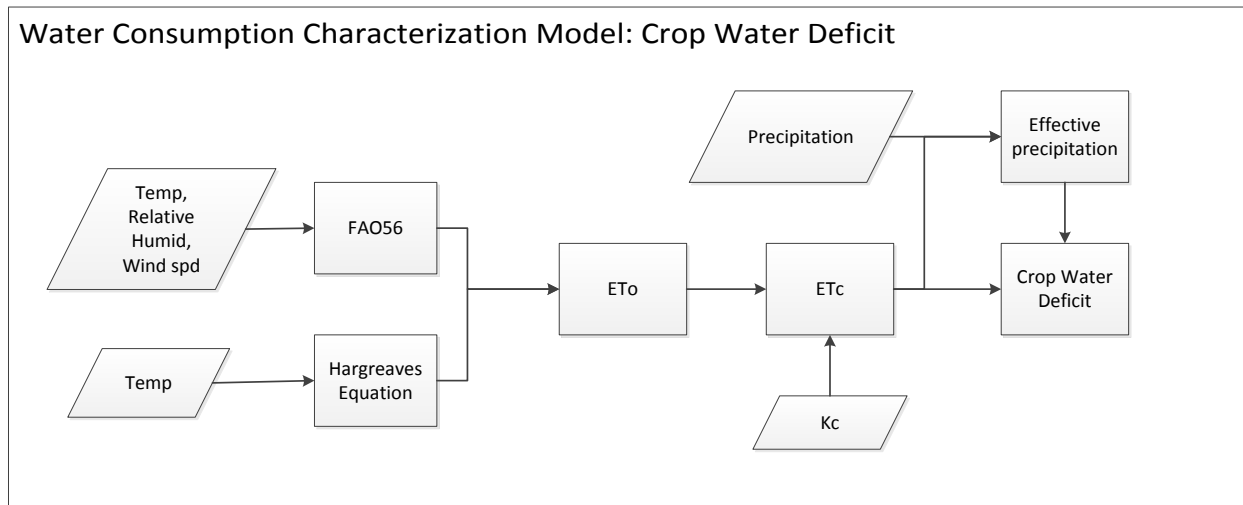


Figure 13: Flow diagram for estimation of crop water deficit

Using these relationships, freshwater consumption is estimated for the production of one kg of a given crop.

Estimates of consumption combine the characterization factors with inventory data representing the:

- the irrigation water applied from surface water sources (m^3/kg)
- the irrigation water applied from groundwater sources (m^3/kg)

- the land area (ha / kg)

Specifically, blue water consumption is estimated by dividing the value of BW (i.e., the result of Equation 22) by the total amount of water applied. The resulting characterization factor can be interpreted as “percentage of applied water consumed per kg of crop produced” (Equation 25). Green water consumption is estimated by multiplying GW (the results of Equation 21) by the land area (and divided by 10) to produce units of m³ / kg (Equation 26).

Equation 25: Characterization factor for blue water consumption, as a function of water applied

$$CF_{blue} = \frac{BW}{W_{app}}$$

Equation 26: Characterization factor for green water consumption, as a function of area

$$CF_{green} = GW * area / 10$$

To complete the interpretation of the freshwater consumption estimates, sensitivity and uncertainty analyses are performed, demonstrated as follows.

3.2 Case study

A preliminary case study was performed to observe the impact of uncertainty and variability on the FAO56 method and the Hargreaves equation for the estimation of freshwater consumption in the production of corn. Estimates of the water applied are based on irrigation and manure applications from the USDA Economic Research Service’s (ERS) Agricultural Resource Management Survey²⁰ (ARMS). Among other crop-state-year combinations, the ARMS data represent corn production in 20 US states over multiple years as summarized in Table 6. The irrigation data are presented as the product of the irrigated area and depth of irrigated water applied by gravity or pressure systems per kg of corn grain produced. The water source is represented as a percentage of irrigated area irrigated from surface or groundwater sources. When the sum of irrigated area for either application type or source does not equal the total irrigated area, the balance is documented as “unspecified” source or application type.

For water applied with manure, because the ARMS data are not available by source, all withdrawals are assumed to be from unspecified sources. The amount of water is estimated dependent upon the state of the manure at application, as either semi-dry or dry, lagoon liquid, or slurry liquid and the additional amount withdrawn is

²⁰ See <http://www.ers.usda.gov/Briefing/ARMS/>

assumed to be zero when the manure is sprayed using irrigation systems. The moisture contents at application are from the Integrated Farm System Model²¹ (IFSM) and are assumed to be 93-95% for lagoon liquid, 80-88% for semi-dry or dry manure, 90-92% for slurry liquid, and 80-85% for instances in which the form was not specified. For both the irrigation and manure data, ARMS represents sampling error as a Relative Standard Error (RSE), estimated from a delete-a-group jackknife resampling routine (J.S. Cooper, Kahn, and Ebel 2011). ARMS data are combined here with crop yield statistics from NASS Quick Stats (NASS 2012) to produce a unit of water from surface, ground, or unspecified water sources per unit of corn (m³/kg).

Table 6: ARMS program states for corn (1996 – 2005)

ARMS program states for corn	Number of years between 1996 and 2005 that are represented
CO	5
GA	2
IA	7
IL	7
IN	7
KS	6
KY	6
MI	7
MN	7
MO	7
NC	6
ND	3
NE	7
NY	3
OH	7
PA	5
SC	1
SD	7
TX	6
WI	7

The RSE in the ARMS data are propagated to the water application estimates through the following rules, as described by Dieck (Dieck, 2006). These rules are solutions to the more general first-order Taylor expansion approximation of the propagation of error (Equation 29). Here, F is some function of independent variables x , and y , for which the errors are known.

²¹ See <http://www.ars.usda.gov/main/docs.htm?docid=8519>

Equation 27: Propagation of error through addition of two variables

$$Z = X + Y; dZ = \sqrt{dX^2 + dY^2}$$

Equation 28: Propagation of error through product of two variables

$$Z = X * Y; dZ = \sqrt{dX^2/X + dY^2/Y}$$

Equation 29: General Taylor approximation of propagation of error

$$SE_F = \left| \frac{\partial F}{\partial x} \right| SE_x + \left| \frac{\partial F}{\partial y} \right| SE_y, \text{ for } F(x, y)$$

Note that some of the RSE values reported by ARMS can be quite high, with some values being greater than 100% which is physically infeasible as it would suggest some estimates of the water applied are less than zero.

Specifically, although the majority of the data have RSE values less than 100%, the range of values in the ARMS irrigation data used here is 84% to nearly 500% of the estimate. The high RSE values can arise as a consequence of using a jackknife on data without explicit calibration of weights (J.S. Cooper, Kahn, and Ebel 2011) and can have a significant impact on the certainty of the subsequent estimates.

Given these estimates of water applied (i.e., given the inventory results), green and blue water consumption is estimated as described in Section 3.1.3, including a sensitivity as summarized in Table 7. Specifically in analyzing sensitivity of freshwater consumption due to changes in reference ET, each independent variable is varied at plus or minus one standard deviation, when known. For use of the ARMS irrigation data in both the FAO56 and Hargreaves methods, the standard deviation is estimated from the RSE based on the jackknife with a sample size of 15. Sensitivity due to the unknown sources of water for irrigation and manure application are estimated by adding each to the maximum estimates for ground and surface water estimates. For the FAO56 method specifically, sensitivity to relative humidity was determined by varying between maximum and minimum average values reported for each month and sensitivity due to wind speed is estimated by ranging from 0 mph, to twice the reported normal wind speed. Also, the ground heat flux (G in Equation 16) was stepped as $G = 0, 0.1 * R_n$ and $0.5 * R_n$ thus varying R_n , the net incoming solar radiation (see Equation 16).

Table 7: Parameters and variables for sensitivity analysis

Parameter	Variable	Range
Reference ET	Maximum temperature	+/- standard deviation
	Minimum temperature	+/- standard deviation
	Relative humidity	Max and min monthly average value
	Wind speed	0 to 2 x average value
	Ground heat flux	0, .1Rn, .5Rn
	Model used	FAO56, Hargreaves equation
	Spatial resolution	256 – 6915 stations
Potential ET	Crop coefficient	Tropics/sub-tropics summer rain
		Sub-tropics winter rain/Oceanic
		Temperate/Boreal
P_{eff}	Depth of water storage	1, 3 (assumed average), 5 inches
	Average precipitation	25 th to 75 th percentile
Irrigation water applied	Groundwater	+/- standard error
	Surface water	+/- standard error
	Unspecified source/manure	from groundwater, from surface water

The variability in P_{eff} is treated the same way in both the FAO56 and Hargreaves methods. It has three independent parameters, potential crop ET, precipitation, and soil depth. Sensitivity of the P_{eff} due to changes in precipitation is estimated by ranging actual precipitation from the reported 25th percentile to 75th percentile, when they are reported. Soil moisture is a highly resolved, stochastic, time dependent variable and is not explicitly modeled in this study, thus it represents a source of uncertainty. Sensitivity to the uncertainty in soil moisture is represented by varying the depth from 1 inch to 5 inches, and using 3 inches as the default value. Given these conditions, the influence of model selection is measured by comparing the results of the FAO56 and Hargreaves equation at the same location, using the same station data based on the root mean square difference (RMSD).

3.2.1 Sensitivity analysis

For the case study, the RMSD of ET_o between the FAO56 and Hargreaves methods was calculated for each station along a twelve-month period, with the maximum RMSD for any station at 2.02 mm/day (stations 23169 in Nevada) and the minimum RMSD at 0.18 mm/day (station 24225 in Oregon). The mean and median RMSD between the two methods was found to be 0.51 and 0.43 respectively with a standard deviation of 0.23 (all in mm/day). These results are in line with what would be expected considering past work validating the Hargreaves equation (Hargreaves and Allen 2003) and are displayed by month in Figure 14. Although these differences are reasonable when estimating daily crop water needs, over a one-month time step, 0.5 mm/day error can accumulate to a 15 mm/month difference.

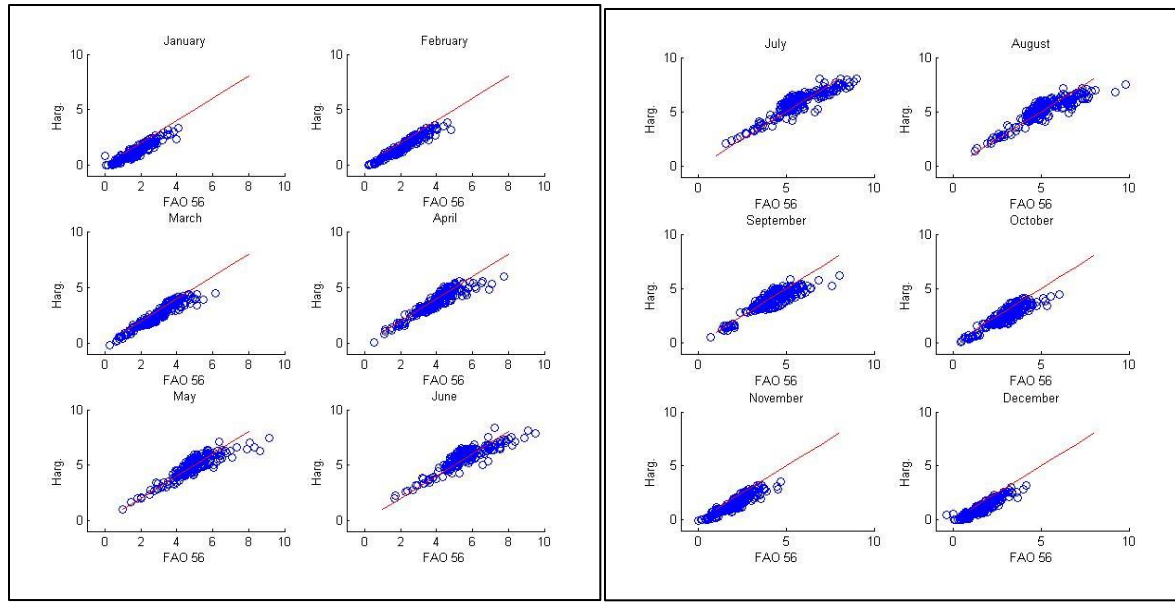


Figure 14: Reference ET₀ using Hargreaves and FAO56, in mm/day

Given these results, the case study estimates of blue water consumption for corn production in the ARMS program states, BW is found not to be sensitive to the crop ET_c. Conservative assumptions were made, such as the rate of water application not exceeding the rate of soil saturation leading to runoff, or the assumption that the depth of application did not exceed soil capacity. Even with these conservative assumptions, we find that for all program states, with the exception of Nebraska, applied water is consistently less than the crop water deficit, suggesting some amount of plant water stress is typical for corn production. For the case of Nebraska, an 8% increase in BW is observed for the *low humidity* case of the FAO56 model estimation, a result not reproduced by the Hargreaves equation. Although it has been suggested that humidity and air temperature are coupled, and thus humidity effects are implicitly included in the Hargreaves Equation (Hargreaves and Allen 2003), in this case, the additional actual ET was not observed.

Conversely, GW is directly affected by the potential ET, as it is a factor in P_{eff}, as well as the limiting factor of P_{eff}. Thus the choice of model directly affects the estimate for green water consumption. Given that sensitivity due to the choice of model is revealed in the estimation of green water consumption, potential ET was modeled using both the FAO56 method and the Hargreaves equation to measure the influence the choice and the accuracy climate models have on overall water consumption inventories.

Using the simpler Hargreaves equation instead of the FAO56 model amounts to a difference of about +/- 2.5%, and up to about 6% for Georgia and Kentucky when compared to the FAO56 estimates. However, Colorado displays an overestimate of about 10% when compared to the FAO56 estimate. In comparison, simpler model results in a decrease in uncertainty due to spatial scale, ranging from about 7% to as much as a 23% reduction in variability, as shown in Table 8 and Figure 15.

Table 8: Comparison of models for estimation of green water consumption

	FAO56		Hargreaves		Change in variability: FAO56 - Hargreaves	
	Under average green water %	Over average green water %	Under average green water %	Over average green water %	Under average green water delta %	Over average green water delta %
CO	67%	38%	60%	27%	7.1%	11%
GA	65%	41%	56%	26%	8.9%	15%
IL	68%	39%	57%	19%	11%	20%
IN	69%	39%	56%	17%	13%	22%
IA	68%	40%	59%	17%	9.4%	23%
KS	73%	38%	64%	18%	9.1%	21%
KY	66%	40%	55%	17%	11%	24%
MI	61%	38%	48%	26%	12%	12%
MN	64%	34%	55%	22%	8.6%	12%
MO	68%	42%	58%	20%	10%	22%
NE	70%	37%	62%	18%	8.0%	18%
NY	62%	38%	48%	23%	14%	15%
NC	64%	36%	53%	26%	11%	10%
ND	70%	36%	63%	18%	7.6%	18%
OH	65%	37%	54%	17%	11%	19%
PA	63%	37%	50%	21%	13%	16%
SC	63%	39%	54%	28%	9.5%	10%
SD	70%	38%	63%	18%	7.1%	20%
TX	73%	39%	68%	25%	5.4%	14%
WI	64%	39%	53%	23%	12%	16%

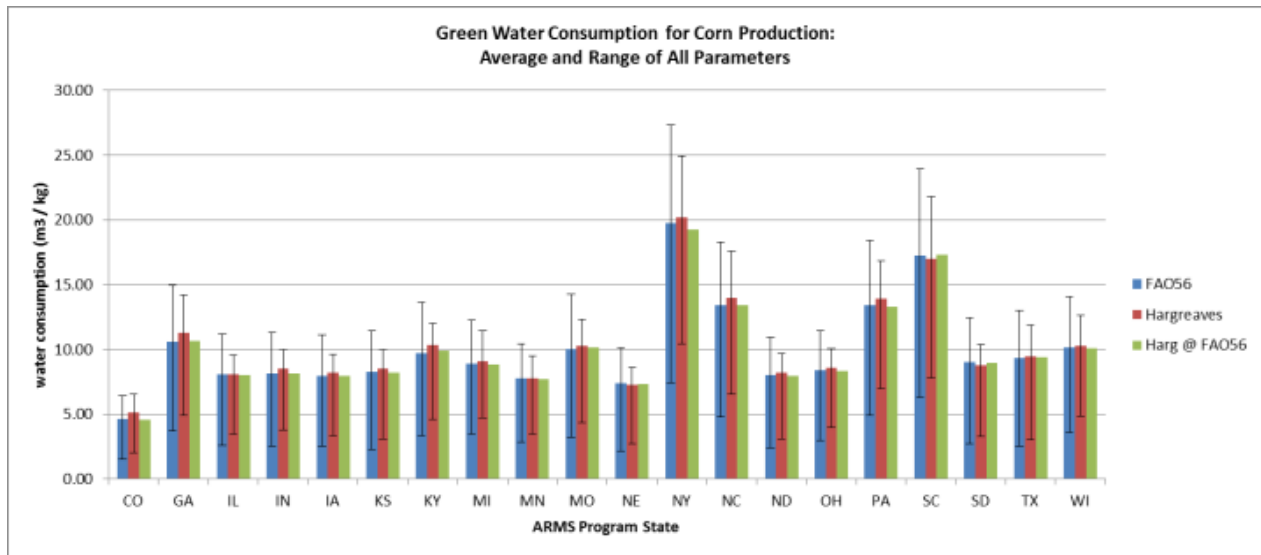


Figure 15: Green water consumption for corn

The sensitivity of green water consumption to individual model parameters was studied by varying each parameter by the value given in Table 7 while keeping all other parameters at their default value. The FAO56 model displayed the largest sensitivity to relative humidity, ranging on average from an almost 60% decrease to nearly 10% increase in green water consumption. These results are presented in Figure 16 and Figure 17.

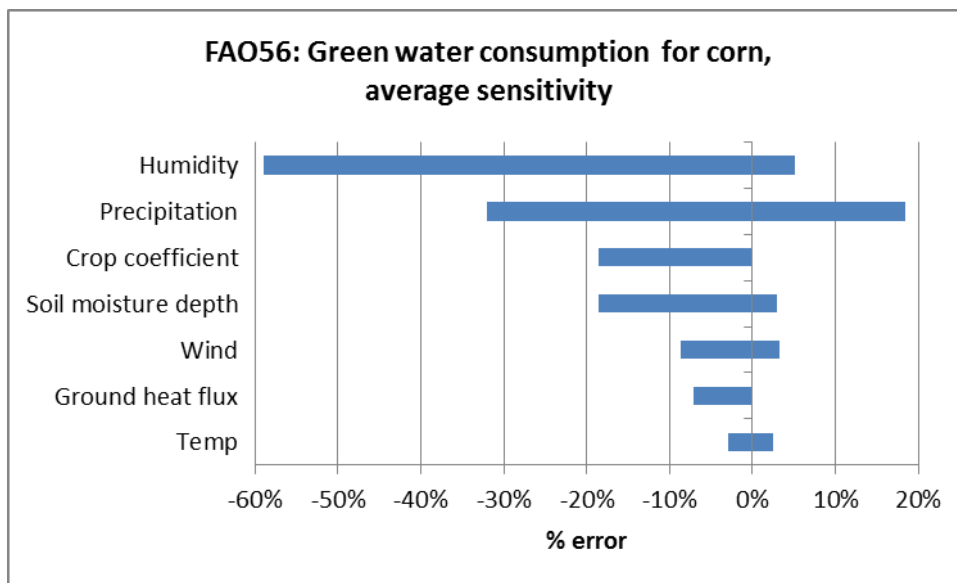


Figure 16: FAO56 green water consumption sensitivity

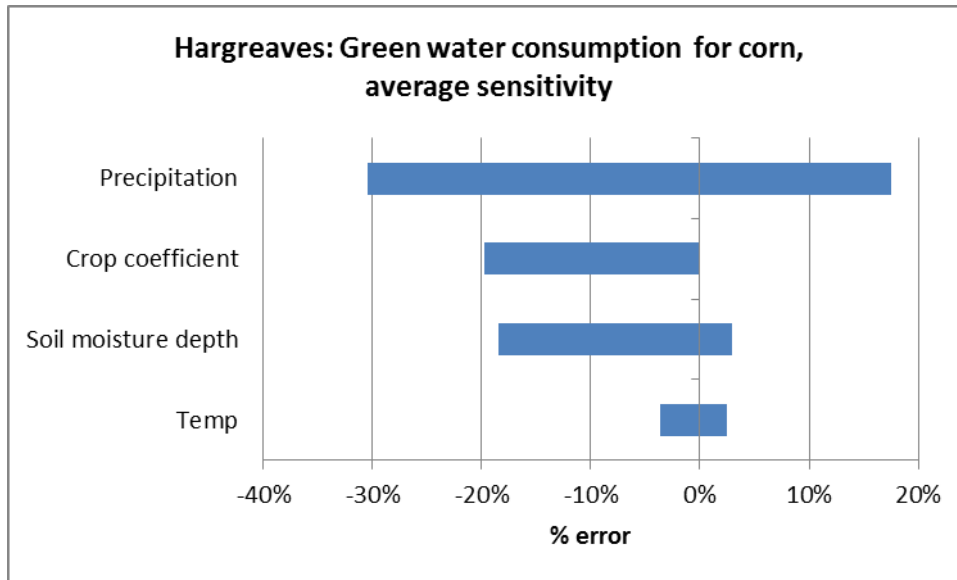


Figure 17: Hargreaves green water consumption sensitivity

Sensitivity due to variability in crop data is revealed in the estimation of blue water consumption. Relative standard error for irrigation application, when known, ranges from 84% to nearly 500% of the estimate. This is not an atypical result, even for original statistics with reasonable reported statistical error (J.S. Cooper, Kahn, and Ebel 2011). However, even with a large uncertainty associated with application data, the range of values within a standard error are less than the CWD calculated using the FAO56 method (Table 9). For program states with a significant amount of water application during crop production, water associated with manure application is a very small component. This suggests that the climate estimates do not affect the quantity of blue water consumed, and corn grown in the ARMS program states experience some amount of water stress during their seasonal life cycle.

Table 9: Irrigation water applied vs. CWD for corn (note: water applied = water consumed in this case)

	Ground water applied	Surface water applied	Unspecified source as irrigation applied	Unspecified source as manure applied	Ground water applied	Surface water applied	FAO56: CWD	FAO56: CWD
	m3/kg prod	m3/kg prod	m3/kg prod	m3/kg prod	RSE (%)	RSE (%)	m3 / kg prod	RSE (%)
CO	2.1E-01	1.1E-01	1.2E-02	3.8E-04	420%	360%	9.0E-01	16%
GA	6.5E-02	3.4E-02	2.8E-03	1.5E-04	--	--	5.5E-01	9%
IL	1.2E-03	--	1.9E-04	5.8E-05	790%	--	4.1E-01	13%
IN	--	--	--	1.0E-04	--	--	4.2E-01	4%
IA	--	--	--	1.7E-04	--	--	3.8E-01	11%
KS	1.8E-01	4.0E-03	6.0E-03	1.6E-05	--	--	6.2E-01	22%
KY	--	--	--	9.7E-05	--	--	4.7E-01	11%
MI	1.5E-03	2.7E-03	6.9E-03	5.5E-04	290%	1000%	5.6E-01	6%
MN	9.9E-04	--	7.3E-05	3.2E-04	--	--	3.7E-01	9%
MO	2.2E-02	--	9.9E-03	2.9E-05	220%	--	5.0E-01	6%
NE	1.9E-01	2.1E-02	7.4E-03	4.1E-05	130%	140%	5.4E-01	19%
NY	--	--	--	4.9E-03	--	--	1.1E+00	9%
NC	--	--	--	2.9E-04	--	--	5.6E-01	21%
ND	--	--	--	4.2E-05	--	--	7.4E-01	12%
OH	--	--	--	2.2E-04	--	--	4.3E-01	7%
PA	--	--	--	2.6E-03	--	--	7.1E-01	9%
SC	--	--	--	--	--	--	7.5E-01	11%
SD	2.5E-03	8.1E-04	3.9E-04	7.4E-05	--	300%	7.3E-01	23%
TX	3.1E-01	9.9E-03	2.3E-02	--	--	--	8.7E-01	27%
WI	3.0E-04	--	1.2E-03	1.7E-03	--	--	4.7E-01	4%

In estimating GW for corn with the FAO56 method, the results can shift by over 60% of the estimate based on variation in average relative humidity, data that is available at only a handful of weather stations in each state.

Consideration must also be given to the lack of spatial resolution when using the climate normal data. As is illustrated by Figure 5, there are only several data points for each state with sufficient data to implement FAO56.

The ERS resource regions illustrate areas with similar crop growth characteristics, and many states are composed of multiple regions. For example, Wisconsin, one of the ARMS corn program states, has 3 resource regions within its borders: one region has three weather stations, one has one station, and one resource regions has no weather stations at all. Estimating ET_c with a simpler model such as Hargreaves equation can greatly improve the spatial resolution, covering a diversity of landscapes.

It should be noted, however, that although the variability in GW is reduced using the Hargreaves equation, it is still quite sensitive to variability in precipitation data. This variability is simply naturally occurring, which stresses the importance of including confidence intervals in LCA results. Furthermore, an understanding of green water

consumption and its role in affecting source recharge must be addressed at a relevant spatial scale. To interpret GW to be a direct impact on water resources is to assume that if the production of that crop were to cease, that the GW would equal zero, or that GW is an additional burden that didn't exist to a local water source before. This is simply not the case, since an alternative ground cover, even a "naturally occurring" one, would also have a non-zero GW value. Additionally, bare soil is a poor medium for water retention, and areas with low vegetation tend to have high runoff rates, at time scales too short for the runoff to recharge water sources. Thus, within the LCA context, GW is meaningless as a stand-alone indicator, or as an indicator to use in a comparative LCA. An appropriate application of the GW indicator is to document the *change* in potential recharge due to the *change* in ground cover and subsequent GW for similar precipitation events.

For corn grown in the ARMS program states, the choice of climate model, and the assumptions made in model implementation, were not found to change the results for BW. This suggests that in practice in the US, corn is typically produced in a state of water stress during at least part of its growth period. Furthermore, an assumption implicit in this study is that water is applied only when a positive CWD exists, and e.g., irrigation applications are timed to maximize the productive use of the water. This assumption does not consider less than optimal management practices such as overwatering, watering at rates in excess of the soil saturation rate, or system losses. Thus, although BW as it is reported here is less than in other studies ((Dominguez-Faus et al. 2009) for example) it is in fact a conservative estimate, as actual BW would likely be lower. The overestimation of BW by some studies is furthered by assuming that $BW \approx CWD$. We find that in practice, water applied can be several times less than what would be required to fully satisfy a crop's water requirement. Furthermore, for states with significant water application, water applied as manure is a minor contributor to consumption compared to water applied as irrigation.

This work has demonstrated that choices in model, study scope, and data availability can have a large effect on freshwater consumption estimates for U.S. corn production. The simple regression model, although producing an accurate expected value, is insensitive to variability in key climate parameters such as relative humidity. Thus the regression equation, a reasonable approach as a back-of-the-envelope tool, is not appropriate for developing LCIA characterization factors. However, to implement a physical model while capturing spatial variability, a higher spatial resolution dataset is required than that provided by the NOAA stations for FAO56. Thus the following

section expands upon this sensitivity analysis for green and blue water consumption with a more in-depth study of contributions to variability and uncertainty, including a wider range of crops.

3.2.2 Uncertainty analysis

3.2.2.1 Methods

The uncertainty analysis builds on the green and blue water consumption sensitivity analysis of the previous section in the following ways:

- Climate data at an 1/8th decimal degree was used
- Represented crops were expanded to include all state-crop combinations in the USDA LCA Digital Commons
- A simplified physical model, the Priestley – Taylor method, was used as a physical, reduced parameter model instead of the Hargreaves equation
- A Monte Carlo sampling procedure was performed to estimate summary statistics of final characterization factors

In addition to corn, the uncertainty analysis was expanded to include eight additional crop types: cotton, oats, peanuts, rice, soybeans, spring wheat, spring wheat excluding durum, and winter wheat. Green water consumption is estimated for all state-crop variables. Blue water consumption for surface and groundwater sources is considered for those state-crops with that type of application. The total list of state-crop variables considered, and the type of water application is presented in Figure 18.

	Corn	Cotton	oats	peanuts	rice	soybeans	spring wheat	spring wheat exc durum	winter wheat
AL		G,P		G,P					
AR		G,V,P			G,V	G,V,P	G		
AZ		G,V,P							
CA		G,V,P			G,V		G,V	G	
CO	G,V,P						G,V,P		G,P
DE							G		
FL				G,P					
GA	G,P	G,P		G,P			G		
IA	G		G			G			
ID							G,V,P		G,V,P
IL	G,P		G			G,P	G		
IN	G					G			
KS	G,V,P		G			G,V,P	G,V,P		
KY	G					G	G		
LA		G,V,P			G,V	G,V,P	G		
MD						G			
MI	G,P		G			G,P	G		
MN	G,P		G			G,P	G		G
MO	G,V,P	G,V,P			G,V	G,V	G		
MS		G,V,P			G,V	G,V,P	G		
MT							G	G	G,V,P
NC	G	G		G		G	G		
ND	G		G			G	G	G	G
NE	G,V,P		G,P			G,V,P	G,P		
NY	G		G						
OH	G					G	G		
OK							G		
OR							G,V,P		G,P
PA	G		G			G	G		
SC	G	G,P							
SD	G,P		G			G	G		G
TN		G				G			
TX	G,V,P	G,V,P	G	G,P	G,V		G,V,P		
VA						G			
WA							G,P		G,V,P
WI	G,P		G			G			

Figure 18: ARMS program states, and the type of water application considered, *G* refers to green water, *V* refers to gravity applied blue water, and *P* refers to pressure applied blue water

The consumption model employed for the uncertainty analysis is the same as was employed for the sensitivity analysis. Green water consumption is estimated as the minimum of either ET_c or P_{eff} , and blue water consumption is the minimum of either CWD or W_{app} (Equation 21 and Equation 22 respectively). The estimation of ET and crop water deficit was performed using two methods, the FAO 56 method (an implementation of the Penman-Monteith equation, Equation 16), and the Priestley-Taylor method. The Priestly – Taylor method was chosen as an alternative simple model to the Hargreaves equation as a way to accurately represent the impacts of model choice on uncertainty characterization. The Priestley-Taylor method is a simplification of the Penman-Monteith equation, replacing the turbulent mass transfer term with a constant. It is predicated on the observation that the contribution of turbulent transfer to total evapotranspiration is often about 25% of the radiation component. It reduces the amount of data required by removing the relative humidity and wind speed components from the Penman-Monteith equation. However, the lack of sensitivity to turbulent transfer of the Priestley-Taylor method will cause an under-estimate in areas with high wind speed/low relative humidity, and an over-estimate in areas with low wind speed / high relative humidity. Estimation of crop ET based upon the Priestley-Taylor method is calculated by Equation 30:

Equation 30: Priestley - Taylor method

$$ET_o = \frac{\alpha * \Delta * (Rn - G)}{\lambda * (\Delta + \gamma)}$$

Where λ is the latent heat of vaporization (MJ/kg), Δ is the vapor pressure-temperature slope (kPa / C), Rn is the net radiation (MJ/m² day), G ground heat flux (MJ/m² day), γ the psychrometric constant (kPa/C), and α a factor 1.26 for most environments (Dingman 2008).

To summarize, both the FAO 56 method and the Priestley-Taylor method require the following data:

- Air temperature (climate data)
- Incoming radiation (climate data)
- Ground heat flux (derived)

In addition, the FAO 56 method requires:

- Relative humidity (derived)
- Wind speed (climate data)

Both methods also require latitude (in estimating incoming radiation), and elevation. The above data requirements were downloaded from the Variable Infiltration Capacity (VIC) model website, hosted at the University of Washington Department of Civil and Environmental Engineering²². The VIC data is gridded to an 1/8 decimal degree, and covers the continental United States and adjacent portions of Canada and Mexico at monthly timesteps. To aggregate the VIC data to the state resolution, a bootstrapping resampling routine was performed to produce estimates and descriptive statistics. Aggregated data was produced for complete state representation, as well as just for cropland within each state, described in section 3.2.2.2 *Data Aggregation*.

As in the preliminary sensitivity analysis, the amount of precipitation contributing to soil moisture is considered the effective precipitation. The effective precipitation attempts to account for the runoff and evaporation as the precipitation event occurs, effects governed by the rate of precipitation, the soil's water capacity, and evapotranspiration potential of the land cover. The method employed here is the SCS method presented in the National Engineering Handbook (NRCS 1993), a regression equation with three independent variables: monthly precipitation, crop evapotranspiration, and soil water capacity, as shown Equation 18.

Soil water capacity is dependent on several variables, including soil porosity and the root depth of the plant coverage. To estimate the variability of soil water capacity at the state level for a variety of crops, a triangular distribution is applied covering a range of crop types, soil types, and stages in crop development. Ranges of soil water capacity for various soil types are given by the United States Bureau of Reclamation (USBR) as amount of water per unit of rooting depth²³. Moisture capacity for various soil types is displayed in Table 10. The USBR provides a range of root zone depths: field crops, grains, and grasses range from 2 to 3 feet below the surface. Thus, water capacity is the product of the soil moisture capacity and the root zone depth, and is represented in this study as a triangular distribution ranging from 1 to 5 inches, with 3 inches as the median value.

²² http://www.hydro.washington.edu/SurfaceWaterGroup/Data/VIC_retrospective/index.html

²³ www.usbr.gov/pn/agrimet/irrigation.html

Table 10: Moisture capacity for various soil classes

Soil texture Class	Moisture Capacity (in/ft)
Coarse sand	0.70
Fine sand	0.90
Sandy loam	1.2
Fine sandy loam	1.5
Loam	1.8
Silt loam	2.0
Clay loam	2.2
Clay	2.4

Monthly precipitation data are downloaded from the VIC database, and aggregated to the state level in the same manner as the other VIC climate parameters according to the method described below. Similarly the estimation of crop evapotranspiration is described both earlier in this section and in previous sections.

3.2.2.2 Data Aggregation

For both green and blue water consumption, to aggregate up to the state level, the VIC grid was imported into an ArcGIS map of the United States, downloaded from the National Atlas²⁴. Cell-to-state assignment was based upon which state contained the centroid of each grid cell. The number of cell centroids in each state and the result of the cell-to-state aggregation are reported in the first column of Table 11.

²⁴ <http://www.nationalatlas.gov/metadata/statesp020.faq.html>

Table 11: Number of Cells in VIC data grid

State	Number of Cells in Vic	Number of Cropland Cells	State	Cells in Vic	Cropland Cells
AL	822	520	NC	803	594
AR	875	621	ND	1376	1324
AZ	1859	510	NE	1374	1340
CA	2722	1092	NH	169	44
CO	1792	1262	NJ	133	102
CT	85	48	NM	1967	633
DC	1	1	NV	1935	264
DE	33	33	NY	886	272
FL	851	650	OH	723	607
GA	939	734	OK	1148	1067
IA	1006	993	OR	1827	591
ID	1563	830	PA	791	390
IL	989	979	RI	16	12
IN	632	606	SC	493	383
KS	1396	1393	SD	1441	1253
KY	683	504	TN	698	490
LA	716	473	TX	4206	3212
MA	150	98	UT	1462	576
MD	181	167	VA	687	402
ME	617	189	VT	171	14
MI	1081	691	WA	1378	766
MN	1629	1026	WI	1048	456
MO	1204	1070	WV	420	102
MS	758	571	WY	1792	663
MT	2899	1629			

To produce descriptive statistics for each state, bootstrap resampling was performed, using the embedded MatLab routine, *bootstrap*. The *bootstrap* routine takes n samples equal to the original sample size, with replacement, from the original sample, and calculates a requested statistic upon the new sample set. The bootstrap resampling was repeated 1000 times for each of the above parameters, for each month, within each state, with the statistical mean calculated and recorded after each replication. The descriptive statistics for each of the parameters for each month-state was then calculated upon the 1000 means. The results of the bootstrap resampling are reported in Supporting_information_2.xlsx.

One of the features of bootstrap resampling, by way of the law of large numbers, is the distribution of the resampled set will converge with the distribution of the original set as the number of replications increases. After the bootstrap resampling, a chi-squared goodness-of-fit test was performed upon the means, to determine how well they fit to a normal distribution. (The results of the chi-squared test and the resulting descriptive statistics are in Supporting_information_2.xlsx).

Noting that some of the continental United States is non-arable and not used for agricultural production, the VIC data grid was masked with the NASA Land Data Assimilation System (NLDAS)²⁵. NLDAS provides frequencies of occurrence of 18 land cover types, by counting the number of each land cover pixel within a cell, and dividing by the total number of cells. Any cell that had a zero occurrence of cropland land coverage was considered to be non-arable, and was removed from the VIC grid. Figure 19 is a map displaying the cells remaining in the study after filtering by the NLDAS land coverage dataset. The NASA LDAS webpage provides access to two data products, an un-adjusted vegetative data set, and one adjusted by season representation of all present coverage types. The unadjusted data set was used here, as the object was to identify locations where no agricultural activity was occurring. The relative frequency adjustment of land cover types was not considered relevant on non-arable land.

²⁵ <http://ldas.gsfc.nasa.gov/nldas/NLDASvegetation.php>

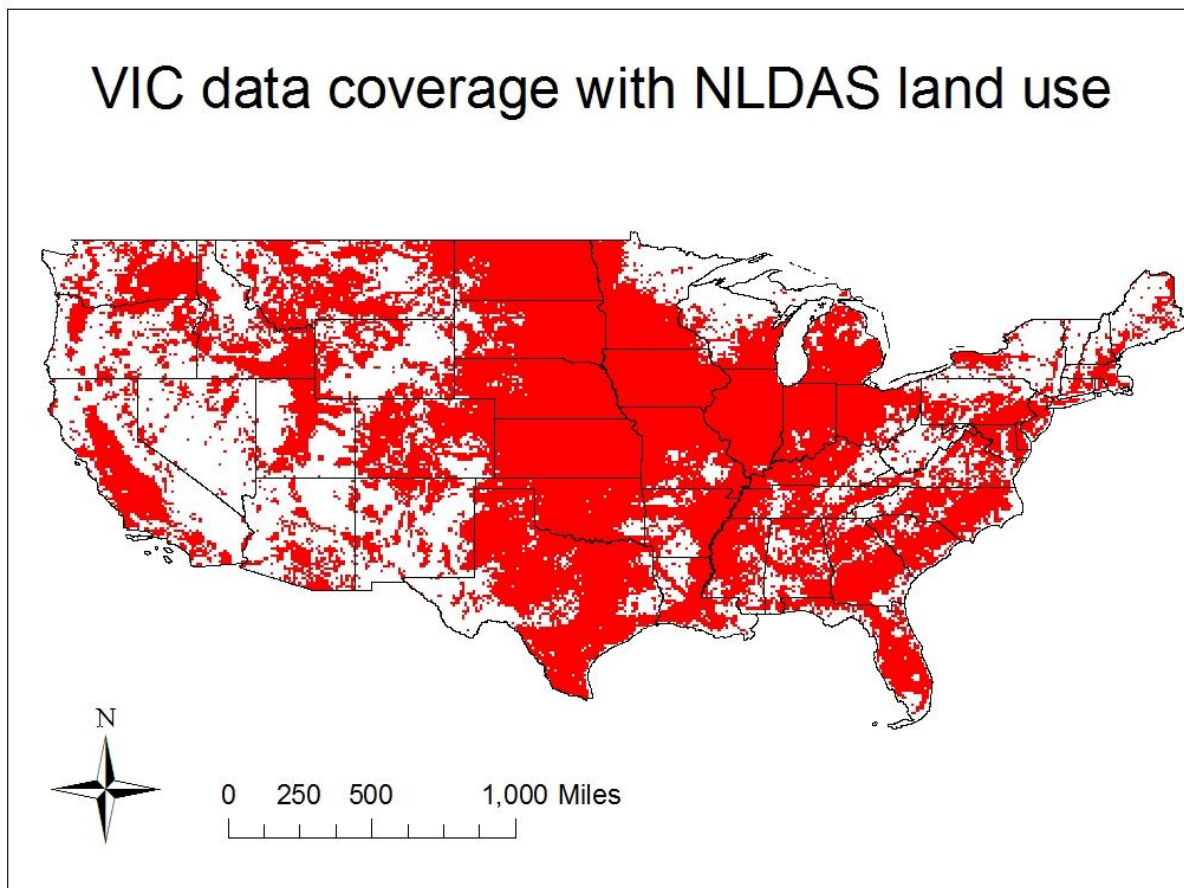


Figure 19: Cells included in study after filtering by land use

3.2.2.3 Water application and yield data

For both green and blue water consumption, water application data are from the USDA ERS ARMS database, as prepared for the LCA Digital Commons (Joyce Smith Cooper, Kahn, and Noon 2012). Again, the ARMS database presents irrigation data as depth of water applied by one of two irrigation technology types: pressure or gravity. For each irrigation technology type, the ARMS database provides a percentage of that water from either surface or groundwater sources. Uncertainty is represented as a Student's *t* distribution with 15 degrees of freedom, except for the 2009 data, which is represented by a Student's *t* distribution with 30 degrees of freedom.

To account for losses due to management practices, the depth of water application reported in ARMS is adjusted by a coefficient. Management practices considered here are variations in conveyance technology used and potential

over-irrigation. To account for losses due to management practices, the amount of applied water that is “available” to the plant/atmosphere system for consumption is adjusted by a coefficient described by a triangular distribution.

Irrigating field crops requires moving water from some source to the point of application. Water that leaves the system and returns to the source through runoff or groundwater percolation is referred to here as conveyance losses. For pressure application, conveyance losses occur due to leaks in pipes, weirs, canals, and intermediate storage facilities. In addition, conveyance losses occur in gravity application systems as water percolates through unlined ditches, trenches, and furrows.

By nature of the technology, water applied by gravity irrigation systems exceeds the irrigation requirements of the crop—some amount of water applied by gravity irrigation will leave the field as unconsumed water. Although pressure irrigation systems offer an improvement in water use efficiency—less water needs to be applied to the field to meet irrigation requirements—pressure systems are still inconsistent in the application of water to the field. Thus, there is some buildup of irrigation water beyond the soil’s holding capacity, and unconsumed water leaves the system.

To account for uncertainty in irrigation management practices, the National Engineering Handbook was used for rule of thumb estimates in irrigation efficiency. In this context, that of the irrigation planner, irrigation efficiency refers to the amount of applied water that is available to the crops to meet water requirements. Irrigation efficiencies are provided for gravity and pressure systems, and for various conveyance losses. The efficiencies are aggregated here as a triangular distribution of possible coefficients. For pressure systems, this coefficient ranges from [0.65,0.9] with an expected value of 0.8. For gravity systems, this coefficient ranges from [0.5,0.9] with an expected value of 0.7.

For yield data, the same source is used as in the preliminary sensitivity analysis. Yield data from NASS does not have uncertainty associated with it. Thus, there is a measure of uncertainty and variability that is not represented in this study, the effects of variability of yield on the results of water consumption. It is recommended that the effects of yield variability be incorporated into further LCA studies, particularly how the magnitude of yield is influenced by changes in farm management practices.

3.2.2.4 Crop coefficients

As is noted in the table of crop coefficients from the case study (Table 5), the value of k_c for corn varies by the length of the growing period, and not by the magnitude of the coefficient. The crop coefficient values provided the Water Footprint of Nations (Chapagain and Hoekstra 2004a) (adapted from the FAO 56 method handbook (Allen et al. 1998)) are resolved to general climate zones, based purely on average temperature. For the detailed work, crop coefficients for all crops in the Digital Commons were customized to the state level by using planting and harvesting dates to adjust the crop coefficient growth periods.

Planting and harvesting dates for the ARMS program crops were collected from the NASS Agricultural Statistics Board, released October 29, 2010²⁶. For planting and harvesting dates, NASS provides three points:

- The **beginning dates** when planting or harvesting is about 5 percent complete,
- The **ending dates** when planting or harvesting is about 95 percent complete,
- And the **most active range** when between 15 to 85 percent of the planting or harvesting is taking place.

In estimating crop evapotranspiration, crop coefficients are resolved to daily timesteps by interpolating the k_c values across growth periods. Coefficients are reported as three values, four growing periods, and a planting date. Values correspond to initial, midpoint, and end periods (k_{ini} , k_{mid} , and k_{end} respectively). The planting date locates when in the year to consider crop evapotranspiration, and the growing periods refer to the number of days within a period—specifically the number of days in the initial, development, midpoint, and end point phases.

The following procedure is employed to adjust growing periods from the NASS growing seasons statistics, based upon the following assumption: the length of the individual growing periods, relative to the total growing season, is independent on the length of the growing period. The fraction of individual growth periods to the total growing season is determined from the values given by (Chapagain and Hoekstra 2004b). To estimate a range of values for length of growing period, a triangular distribution for the planting and harvesting dates is estimated from the NASS statistics (see Supporting_information_1.xlsx). The expected median planting date is estimated to be the average between the beginning and end of the “most active” period, when 15% to 85% of the planting occurs. The beginning of the planting period is a linear extrapolation from the 5% to 15% activity dates. Similarly, the last day

²⁶ <http://usda.mannlib.cornell.edu/MannUsda/viewDocumentInfo.do?documentID=1251>

of planting is a linear extrapolation from the 85% to 95% activity dates. The triangular distribution for possible planting dates is then developed from the extrapolated beginning date to the estimated median, to the extrapolated end date. Although there is some uncertainty associated with the extrapolation of planting dates from available data, it is an approach that can be applied consistently, and it is assumed the influence of outliers in this case is negligible. The preceding process is repeated with the harvesting dates, to develop two triangles of activity ranges, describing the total length of the growing crops' season. The deterministic values k_c from (Chapagain and Hoekstra 2004b) are displayed below in Table 12.

Table 12: Crop coefficients, as reported from (Chapagain and Hoekstra 2004b)

	Corn	Cotton	Wheat, spring and durum	Soy	Wheat, winter	Oats	Rice	Peanuts
kc_ini	0.300	0.350	0.700	0.400	0.350	0.300	0.050	0.400
kc_mid	1.20	1.20	1.15	1.15	1.20	1.15	1.20	1.15
kc_end	0.500	0.600	0.300	0.500	0.600	0.250	0.600	0.600
L_ini	30.0	30.0	15.0	20.0	20.0	15.0	30.0	35.0
L_dev	40.0	50.0	25.0	30.0	60.0	25.0	30.0	45.0
L_mid	50.0	60.0	50.0	60.0	70.0	50.0	60.0	35.0
L_end	30.0	55.0	30.0	25.0	30.0	30.0	30.0	25.0
P_date	136	153	136	153	320	136	167	183

3.2.3.5 Monte Carlo estimation and uncertainty analysis

To produce a set of estimates of freshwater consumption, 1000 random samples were drawn for each required parameter for each state-crop combination. The probability distributions, associated estimates, and the data sources for each parameter are outlined in Table 13. Each parameter contributes to estimates of ET_o , ET_c , effective precipitation, or blue water consumption. For each parameter, a sample was drawn, and the value of that sample was used to calculate a particular instance of each estimate. Thus, in the course of the Monte Carlo procedure, 1000 instances for each estimate were produced.

For the climate parameters derived from the VIC database, samples were drawn from a normal distribution described by the summary statistics developed from the bootstrap resampling. Ground heat flux, net radiation, and temperature are used to estimate ET_o for both the Priestley – Taylor and FAO56 methods. Wind speed and relative humidity are used to estimate ET_o for the FAO56 method exclusively. Crop coefficients are used to calculate ET_c

for both models, precipitation and soil water capacity are used to estimate the effective precipitation, and the depth of water application and the irrigation management data are used in the estimates of blue water consumption.

Random samples for each parameter were drawn once, and saved to disk. For the sensitivity analysis, green water consumption and blue water consumption from surface and ground water sources were calculated using the randomly drawn samples for each of the following parameters while using the expected values for all others the following scenarios:

- Ground heat flux
- Net radiation
- Temperature
- Wind speed
- Relative humidity
- Crop coefficient
- Precipitation
- Water application

The correlation analysis was performed to determine how models differ in their sensitivity to each of the parameters listed above. To determine the correlation between results for the FAO 56 and Priestley – Taylor model, the correlation coefficient was determined using the MatLab function, *corrcoef*. The *corrcoef* function calculates the correlation coefficient of two sets of data:

Equation 31: Correlation coefficient

$$R(i, j) = \frac{Cov(i, j)}{\sqrt{Var(i)Var(j)}}$$

The value of R in Equation 31 is the correlation coefficient defined as the covariance between the two samples, divided by the product of the standard deviations of the two samples. Also known as the *Pearson product – moment coefficient*, it is a measure of the linear dependence between the two models. The value of R ranges from -1 to 1: a value of -1 implies the data are negatively associated, 1 implies the data are perfectly dependent, and a value of 0 implies there is no relationship between the two models. Thus, the relevance of the sensitivity to model selection

can be quantified by the correlation coefficient. That is, a highly sensitive parameter that also exhibits a correlation coefficient close to 1 does not impact the results of model selection uncertainty on the characterization factor.

Table 13: Parameters for sensitivity analysis

Parameter	Distribution	Estimate	Data Source
Ground heat flux	Normal	ETo: FAO56, Priestley - Taylor	(Maurer et al. 2012)
Net radiation	Normal	ETo: FAO56, Priestley - Taylor	(Maurer et al. 2012)
Temperature	Normal	ETo: FAO56, Priestley - Taylor	(Maurer et al. 2012)
Wind speed	Normal	ETo: FAO56	(Maurer et al. 2012)
Relative humidity	Normal	ETo: FAO56	(Maurer et al. 2012)
Crop coefficient	Triangular	ETc	(Chapagain and Hoekstra 2004b), (NASS 2010)
Precipitation	Normal	Effective precipitation	(Maurer et al. 2012)
Soil water capacity	Triangular	Effective precipitation	(NRCS 1993)
Water application	Student's t	Blue water consumption	(“ARMS, Farm Economy” 2010)
Irrigation Management	Triangular	Blue water consumption	(NRCS 1993)

3.2.2.6 Results

Green water consumption.

Sensitivity to model choice

For all of the state-crop estimates, the Priestley-Taylor method underestimated the FAO56 method for green water consumption (see *cumulative_plots.zip* in the supplemental information for complete CDF plots). To determine the statistical significance between the two models, a 2 variable t – test was performed on the characterization factors.

The null hypothesis, that the two datasets have the same mean and variance, was rejected for each of the state-crop green water consumption estimates. Furthermore, the t-test rejected the null hypothesis for all of the individual parameters in the sensitivity analysis. Thus, the two models produce what can be considered statistically different estimates of green water consumption.

To estimate the impact of variability of individual parameters on estimates between the two models, the average absolute difference is taken between the characterization factors estimated by FAO 56 and Priestley – Taylor. The average absolute difference ranges from 1% to 29% of the FAO 56 estimate across the state-crop variables, with an average value of 11%. For individual state-crop variables, there is little variation in difference between the models across the individual parameters—that is, across the various parameters, the absolute difference between the two models ranges from 0.08% to 2.71%. Thus for green water consumption, the choice of model introduces a near

constant bias that isn't particularly sensitive to any one parameter. The complete results of sensitivity to model selection are displayed in Supporting_information_1.xlsx.

Oats grown in Texas exhibits the largest bias of all the state-crop variables, with an average of 27% difference between the FAO56 estimate and the Priestley-Taylor estimate. This bias amounts to roughly 1.5 m³/kg of oats grown in Texas. From inspection of Figure 20, for oats grown in Texas the Priestley-Taylor method underestimates the FAO56 method by roughly 1 standard deviation. Of the 112 state-crop variables studied here, twenty-six exhibit an absolute difference of at least 15% of the FAO56 estimate (Table 14). Of those 26, all but three are spring wheat (with Texas oats, North Carolina soybeans, and Virginia soybeans included).

Table 14: Spring wheat, absolute difference between FAO56 and Priestley - Taylor

State	Crop	% difference of FAO56	Absolute difference (m ³ /kg)
TX	oats	27.0%	1.60E+00
LA	wheat spring	24.4%	4.13E-01
OK	wheat spring	22.5%	1.27E+00
TX	wheat spring	21.6%	8.97E-02
MS	wheat spring	21.3%	5.63E-01
AR	wheat spring	20.2%	5.86E-01
GA	wheat spring	20.1%	1.09E+00
KS	wheat spring	19.7%	1.05E+00
CA	wheat spring exc durum	19.6%	1.09E-01
NE	wheat spring	18.8%	4.49E-01
CO	wheat spring	18.8%	3.43E-01
NC	wheat spring	18.6%	1.59E-01
KY	wheat spring	18.3%	1.18E+00
MO	wheat spring	18.3%	7.10E-02
IL	wheat spring	18.3%	3.81E-01
NC	soybeans	18.2%	3.73E-01
OH	wheat spring	17.7%	7.94E-02
CA	wheat spring	17.6%	1.93E+00
ND	wheat spring	17.1%	3.68E-01
MN	wheat spring	17.0%	6.61E-01
SD	wheat spring	17.0%	1.34E-01
PA	wheat spring	16.9%	8.55E-02
MI	wheat spring	16.4%	3.36E-01
MT	wheat spring	15.9%	4.44E-01
WA	wheat spring	15.8%	9.26E-02
VA	soybeans	15.8%	1.32E-01

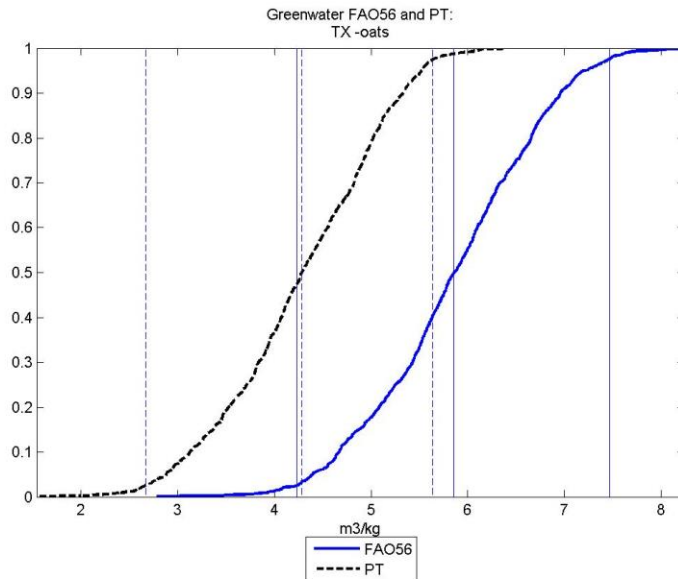


Figure 20: CDF of green water characterization factor for oats grown in Texas

To determine if location alone is enough to determine the level of variability between models, the results were aggregating by crops to the state level. Most of the program states exhibit little consistency of difference between models. The maximum absolute difference for states ranges from 10% (Arizona) to 26% (Texas). The minimum absolute difference ranges from 2.1% (South Dakota) to 22.5% (Oklahoma). The level of model variability across crops within a state can be characterized by the variation between maximum and minimum absolute difference, as displayed in Table 15. States with a zero difference value can be disregarded as states with only a single crop represented (Arizona, Delaware, Florida, Maryland, Oklahoma, and Virginia). Of those states that have more than one crop, the variation in absolute difference ranges from 0.7% (Indiana) to 23.3% (Texas). As low variation in absolute difference suggests location influences the sensitivity to model selection, the states with the smallest variability are identified as Alabama, Indiana, South Carolina, and Tennessee (with 2%, 0.7%, 3.5%, and 6.4% variation respectively). However, though these four states exhibit low variability of model sensitivity across crops, they are amongst the lowest of the total sensitivity to model choice, (with a maximum difference of 10.7%, 11.5%, 11.5%, and 13.9% respectively, the lower third in model sensitivity of all states).

Table 15: Difference in model sensitivity, aggregated by state, as % of estimate of FAO56

	State	Maximum	Minimum	Difference
1	AZ	10%	11%	0.0%
2	AL	10%	8.7%	2.0%
3	FL	11%	11%	0.0%
4	IA	11%	2.5%	8.4%
5	SC	12%	5.0%	6.5%
6	IN	12%	11%	0.7%
7	NY	12%	3.1%	9.0%
8	DE	13%	13%	0.0%
9	WI	13%	2.1%	11%
10	TN	14%	11%	3.4%
11	MD	14%	14%	0.0%
12	OR	15%	3.7%	11%
13	ID	15%	3.8%	11%
14	VA	16%	15%	0.0%
15	WA	16%	3.4%	12%
16	MT	16%	3.2%	13%
17	MI	16%	2.4%	14%
18	PA	17%	2.2%	15%
19	SD	17%	2.1%	15%
20	MN	17%	2.5%	15%
21	ND	17%	3.3%	14%
22	OH	17%	10%	7.4%
23	IL	18%	2.7%	16%
24	MO	18%	8.4%	9.9%
25	KY	18%	8.0%	10%
26	NC	19%	7.2%	11%
27	CO	19%	3.6%	15%
28	NE	19%	2.9%	16%
29	CA	20%	11%	9.0%
30	KS	20%	3.8%	16%
31	GA	20%	5.2%	15%
32	AR	20%	7.1%	13%
33	MS	21%	6.7%	15%
34	OK	23%	22%	0.0%
35	LA	24%	3.4%	21%
36	TX	27%	3.7%	23%

Similarly, the results of model selection are aggregated by states to each of the ARMS program crops. Sensitivity results aggregated by crop show winter wheat having the least difference between models across states, just 1.4% of the FAO56 estimate, however winter wheat also has low difference between models, ranging from 2.4% to 3.8%. Cotton and rice also exhibit somewhat consistent difference between models across states, ranging from 8.3% to 12.8%, a difference of about 4.5% of the FAO56 estimate (Table 16). However, like the state aggregation, crops exhibiting low variation are crops with small absolute differences, suggesting that crop selection itself is not necessarily an indicator of sensitivity to model selection.

Table 16: Difference in model sensitivity, aggregated by crop, as % of estimate of FAO56, sorted by maximum variability

	Crop	Maximum	Minimum	Difference
1	winter wheat	3.8%	2.4%	1.4%
2	rice	11%	3.4%	7.2%
3	cotton	13%	8.3%	4.5%
4	corn	14%	5.0%	9.4%
5	peanuts	15%	11%	3.9%
6	soybeans	18%	7.2%	11%
7	wheat spring exc durum	20%	3.2%	16%
8	wheat spring	24%	13%	11%
9	oats	27%	2.1%	25%

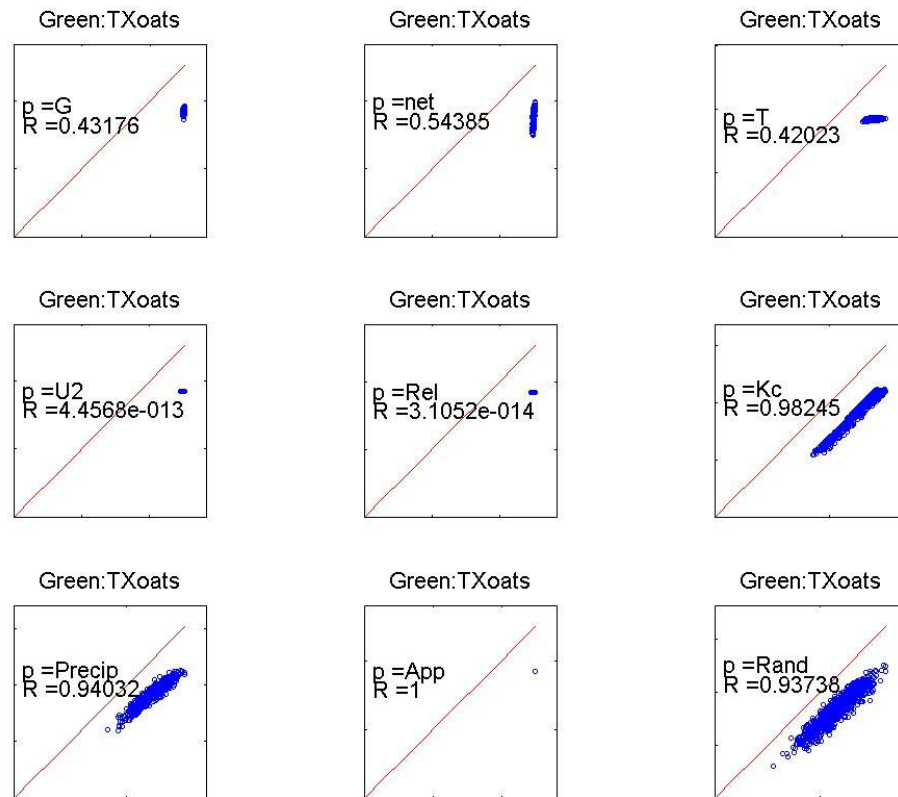


Figure 21: Green water consumption of oats grown in Texas, FAO56 (x – axis) vs. Priestley-Taylor (y-axis)

Parametric Sensitivity

The following procedure was performed to test the sensitivity of the results to the overall estimate. For the individual parameters, the 97.5% estimate and the 2.75% estimate were divided by the expected value from the full Monte Carlo estimate, to produce the 95% confidence interval sensitivity range as a percentage of the expected characterization factor, according to Equation 32.

Equation 32: Estimate of sensitivity of parameter to expected value

$$S_{95\%} = \left[\frac{\mu_p - E_{2.75}}{\mu}, \frac{E_{97.5} - \mu_p}{\mu} \right]$$

Where, μ_p is the average value of the sensitivity estimate, μ is the expected value of the characterization factor; $E_{2.75}$ and $E_{97.5}$ are the 2.75% and 97.5% expected values of the individual parameter sensitivity results. Thus, the

sensitivity analysis gives the lower and higher bounds of the 95% confidence interval of the individual parameter sensitivity, scaled to the expected value of the total characterization factor.

For both models, green water consumption is most sensitive to variation in precipitation and crop coefficient. The average range of sensitivity over the 95% confidence interval for the FAO56 method is displayed in Figure 22, and for Priestley-Taylor in Figure 23. On average, the FAO56 method varies from -11% to 17% due to variation of precipitation data, and varies from -8% to 16% for crop coefficients. The Priestley-Taylor method varies on average from -19% to 15% for precipitation, and from -15% to 15% for crop coefficients.

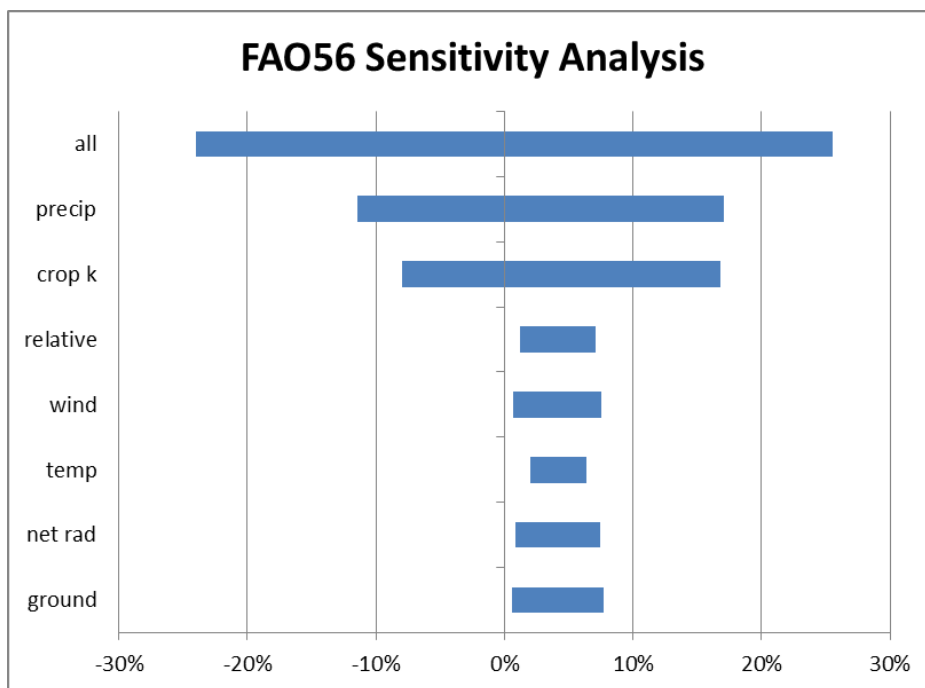


Figure 22: FAO 56 parametric sensitivity for green water consumption

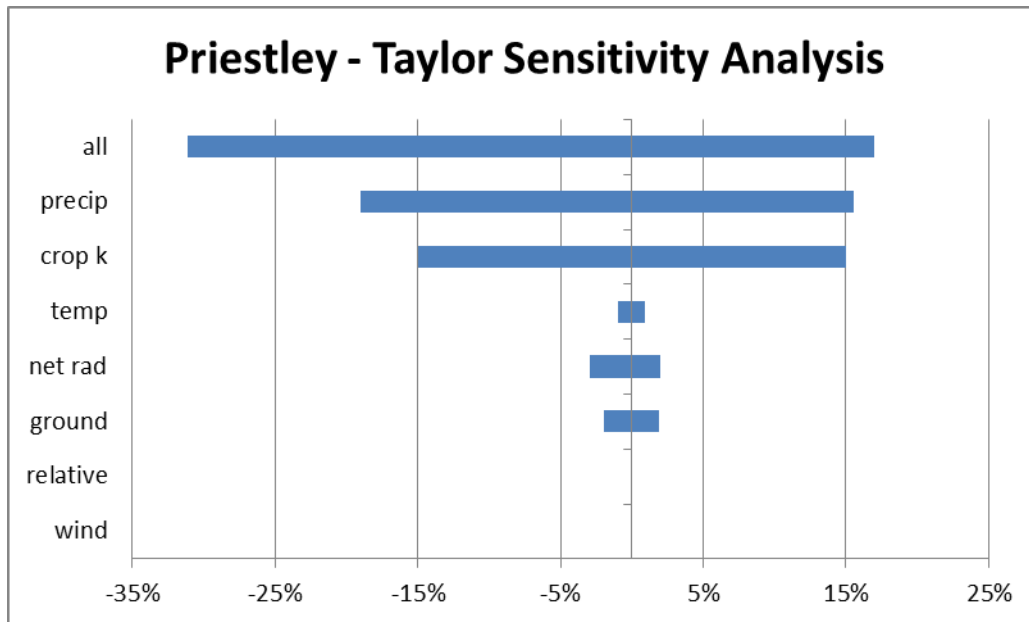


Figure 23: Priestley - Taylor Sensitivity Analysis for green water consumption

For individual state-crop variables, sensitivity to precipitation and crop coefficients can be much higher. Sensitivity to variation in precipitation of the FAO56 method ranges from 66% of the expected value at maximum (spring wheat grown in Delaware), to 17% at minimum (peanuts grown in Texas). For all state-crop variables, the Priestley – Taylor method is slightly more sensitivity to variability in precipitation data, with a range of 74% for Delaware spring wheat, and 26% for Texas peanuts (Figure 24). For crop coefficients, the sensitivity of the FAO56 method ranges from 58% for soybeans grown in North Carolina, to 2.2% for Montana spring wheat. Similarly, the Priestley-Taylor method is also more sensitivity to changes in crop coefficient, with a range of 76% for North Carolina soybeans, to 7% for Montana spring wheat (Figure 25).

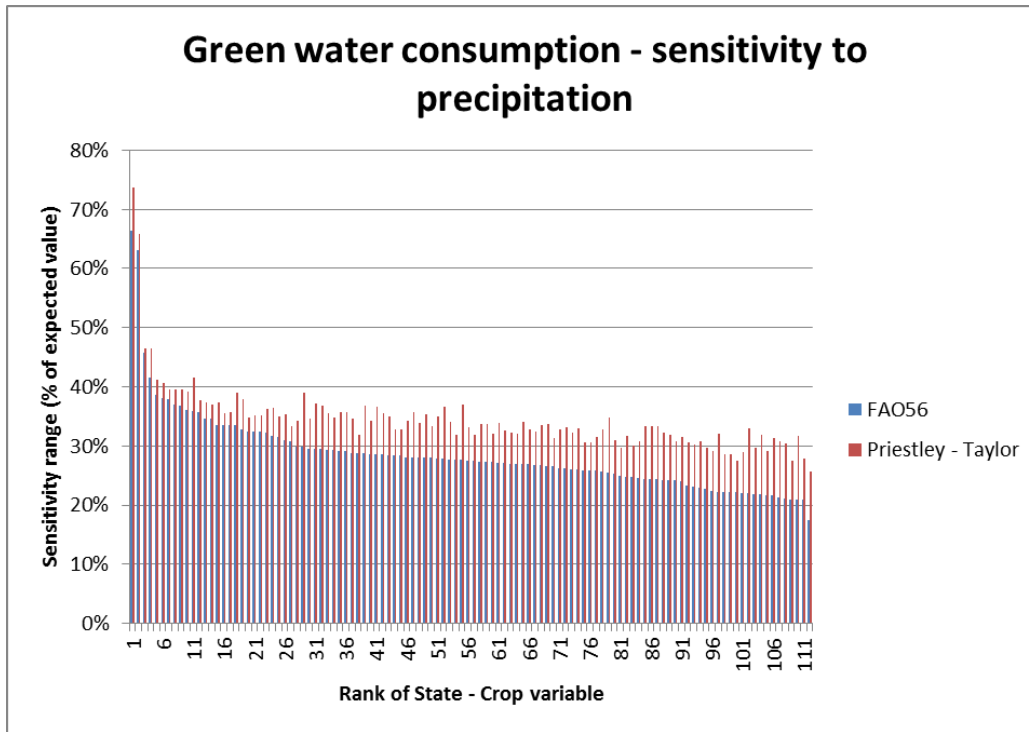


Figure 24: Green water consumption sensitivity to precipitation variability.

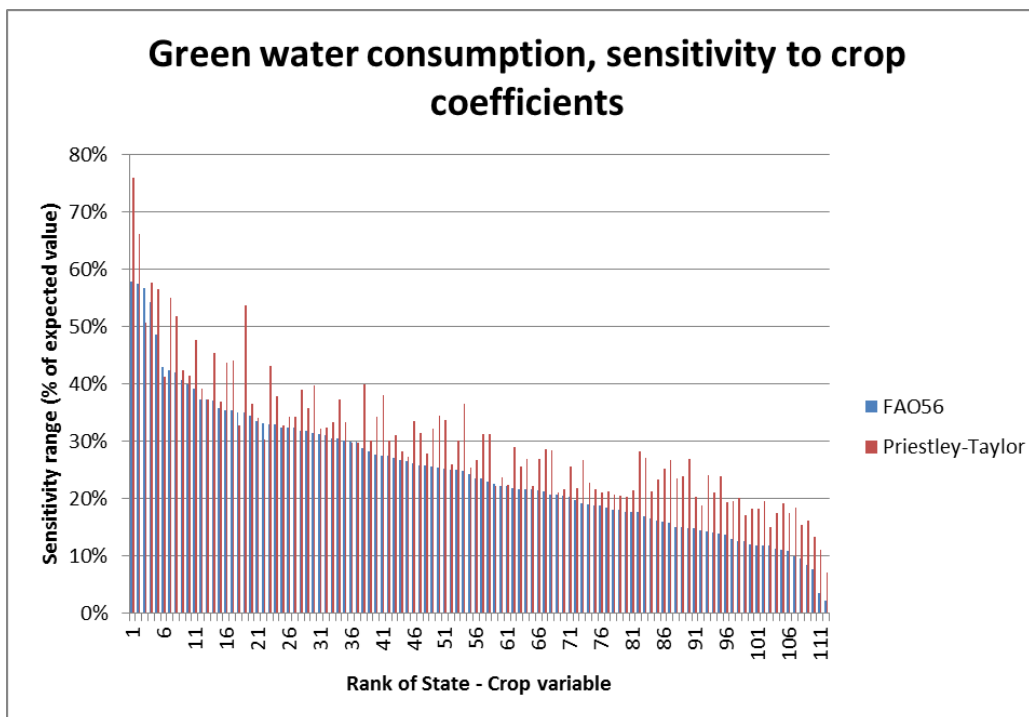


Figure 25: Green water consumption sensitivity to variation in crop coefficients

For each of the results of the sensitivity analysis, a χ^2 goodness-of-fit test was performed, to test how well the green water consumption estimates fit a normal distribution.

By calculating the correlation coefficient between the characterization factors estimated with the two models, the nature of the difference between the results can be characterized. A strong correlation between the two models displays a mutual sensitivity to the parameter being varied, and the difference between the two models can be considered a bias. A lack of correlation between the two models may represent important variability of the parameter that is not being captured by one of the models.

The full random estimates of green water consumption between FAO56 and Priestley-Taylor are strongly correlated for all state-crop combinations studied. The weakest correlation between the two estimates was found for spring wheat grown in Louisiana, which had a correlation coefficient of 0.88. Of the 112 state-crop variables studied here, 73% have a correlation coefficient of .95 or higher, and 99% have a correlation coefficient of at least .90. Thus it can be said that green water consumption estimated by FAO56 and the Priestley-Taylor method are strongly correlated, and the difference between the two models can be considered a bias, and not a random variation.

Blue water from surface sources

Sensitivity to Model Selection

For the 54 state-crop variables with blue water consumption from surface water sources, there is a statistically significant difference between the FAO56 method and the Priestley-Taylor method for 52 of them. Two state-crop variables exhibited no statistically significant difference between the two models: spring wheat grown in California and spring wheat grown in Nebraska. The absolute difference between the results of the two models was 0.43% and 0% respectively.

The absolute difference for the 51 statistically significant state-crop variables ranged from a minimum of 0.54% for Arizona cotton, to 15.2% for Michigan corn. The average difference between the two models is 6%. Estimates of surface water consumption for individual state-crop variables show a wider range of absolute difference across parameters than green water consumption. The average absolute difference is 4% across parameters for individual state-crop variables, and ranges from a minimum of 0.54% for Mississippi rice, to 15% for Minnesota corn. Thus, the level of impact due to model choice varies on a state-crop variable basis.

Nebraska spring wheat is the only state-crop variable that exhibits no variability of surface water consumption due to model choice. The estimation of surface water consumption is sensitive only to the amount of irrigation water applied to the field (Figure 26), and the results estimated by both models are perfectly correlated. As is illustrated in Figure 27, the highest extreme value of surface water application is below the lowest extreme value of crop water deficit so blue water consumption is limited by the amount of water application. Thus the estimation of surface water consumption is independent of the estimation of crop water deficit, and is entirely insensitive to climate parameters and choice of model for estimation ET_o .

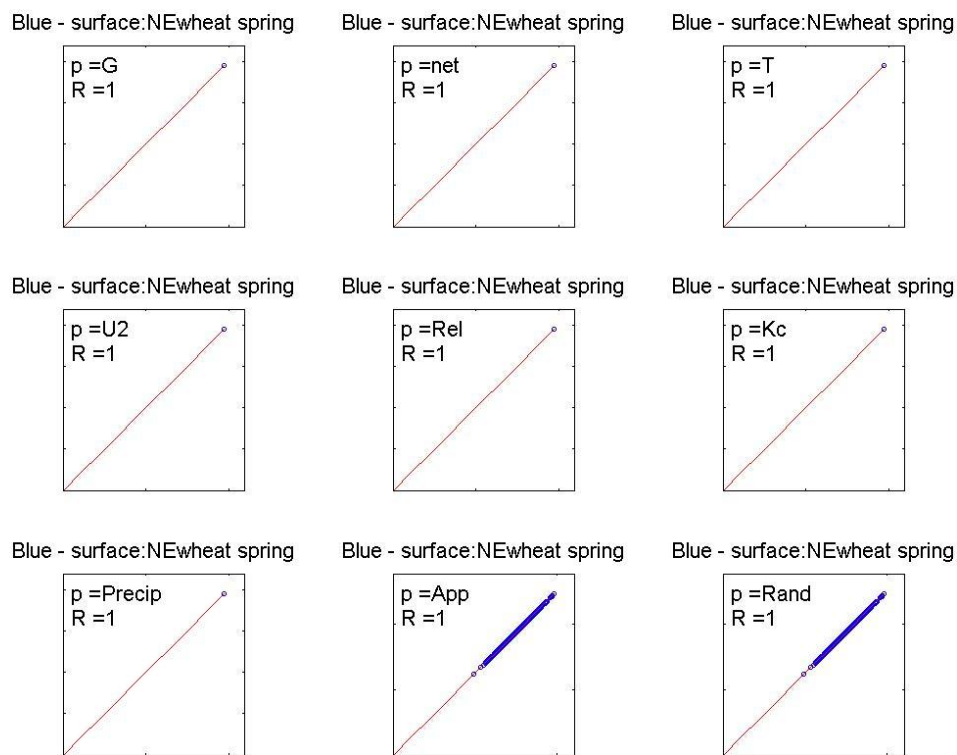


Figure 26: Correlation of FAO56 and Priestley - Taylor for Nebraska spring wheat

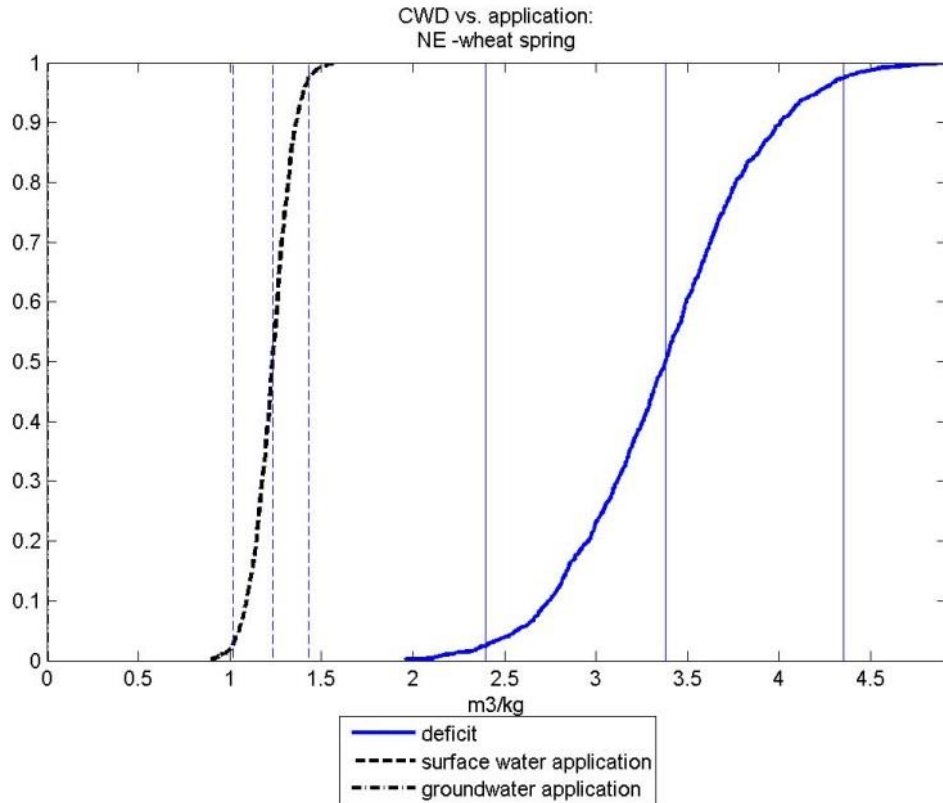


Figure 27: Cumulative results of crop water deficit and surface water application for spring wheat grown in Nebraska – FAO56

In contrast, consumption of surface water for rice grown in California is dependent on both the amount of water applied and the crop water deficit, thus the sensitivity of variability in both management practices and climate data are compounded. The cumulative results for surface water consumption is displayed in Figure 28, note median crop water deficit is within a standard deviation of the median surface water application. The scatter plots of correlation between the two models (Figure 29) illustrate the effect of interaction between water application and crop water deficit.

Although all parameters in the estimate of surface water consumption for California rice correlate well between the two models, elements of non-normality are evident in the plots of temperature, crop coefficient, precipitation, and water application. For example, in the correlation plots of parameters temperature, crop coefficient, and precipitation (parameters describing crop water deficit), the scatter plots display a well correlated, random like pattern below a certain threshold at which point only the Priestley-Taylor estimate continues to increase. This

threshold is the point where the characterization factor shifts from being crop water deficit limited to water application limited: the upper end of the FAO56 estimate is limited by the amount of water available, while the Priestley – Taylor method, which underestimates ET_o , is still water deficit limited, illustrated by the straight vertical lines in the FAO56 vs. PT plots.

In the correlation plot of water application the transition from crop water deficit limited to application limited at the point where the scatter plot maps a horizontal line. Below this point, both models are limited by water application, and the parameter sensitivity is perfectly correlated and equivalent between the two models. At the transition point, the Priestley – Taylor method is limited by the maximum estimate of crop water deficit, while the water consumption estimate from the FAO 56 method continues to rise.

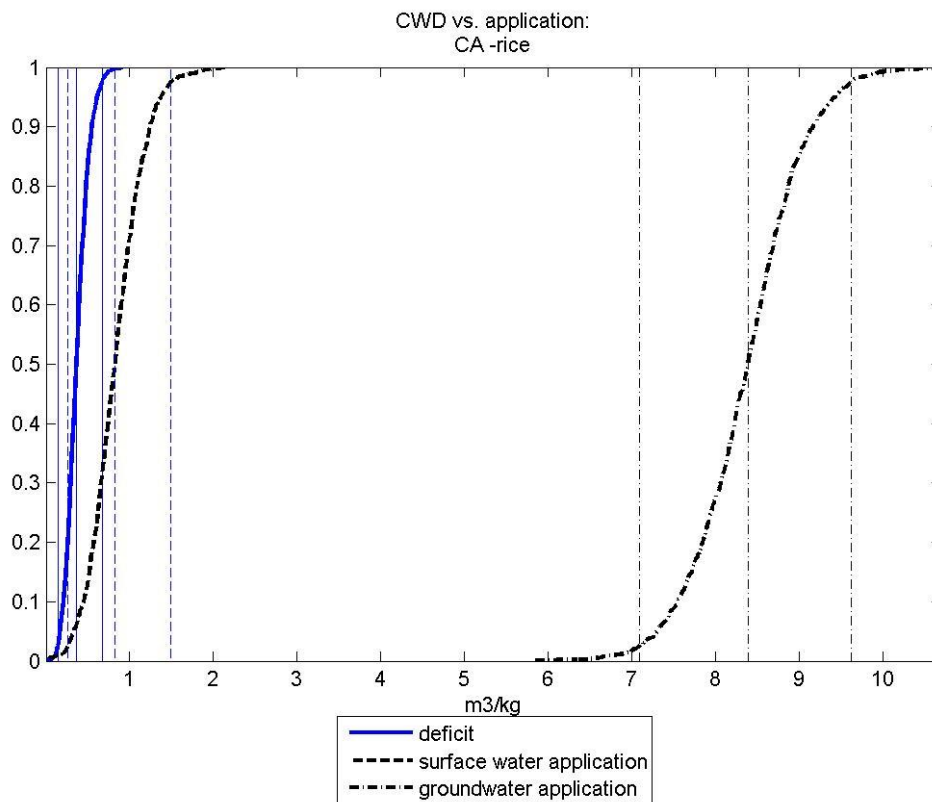


Figure 28: Cumulative results of crop water deficit and surface water application for rice grown in California – FAO56

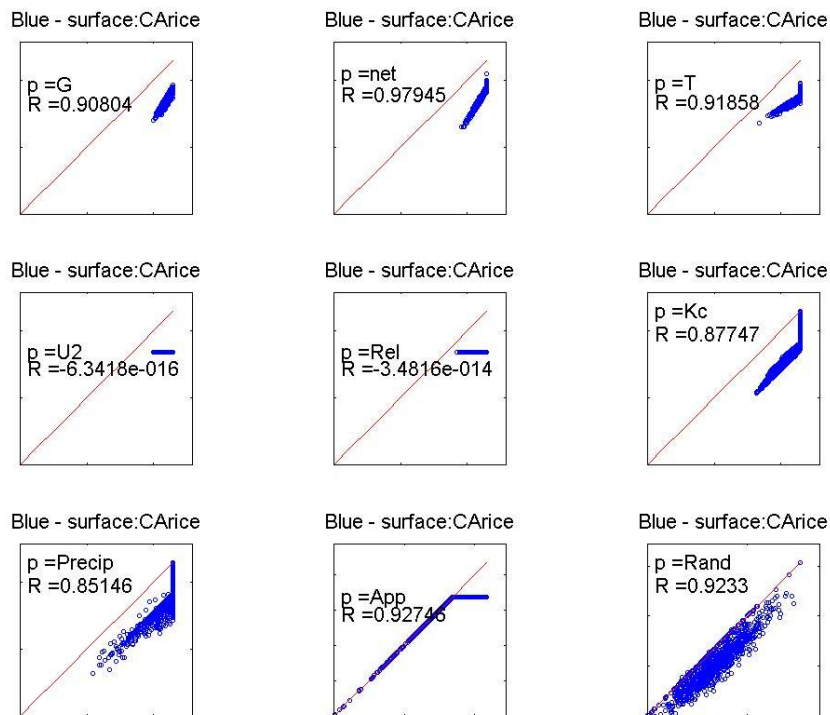


Figure 29: Correlation of FAO56 (x-axis) and Priestley – Taylor (y-axis) for California rice

Parametric Sensitivity

Sensitivity to individual parameters was analyzed with the same procedure used for green water consumption, averaging the range of estimates across all state-crop variables. Average sensitivity of FAO56 estimates to model parameters ranges from 18% for water application to 50% for precipitation. Priestley – Taylor estimates range from 17% for water application to 50% for precipitation (Table 17). For both methods, oats grown in Nebraska exhibits the most sensitivity to parametric variability, with a 400% range in estimates for climate parameters, and 50% range in water application parameters (Figure 30). Overall variation for surface water consumption for Nebraska oats ranges from 13% to 82% with an average of 49%. The average difference between the two methods for the estimation of surface water consumption for Nebraska oats ranges from 1.5% to 3.5% of the estimate, a marginal difference between the two models that show strong correlation for all parameters, besides wind speed and relative humidity.

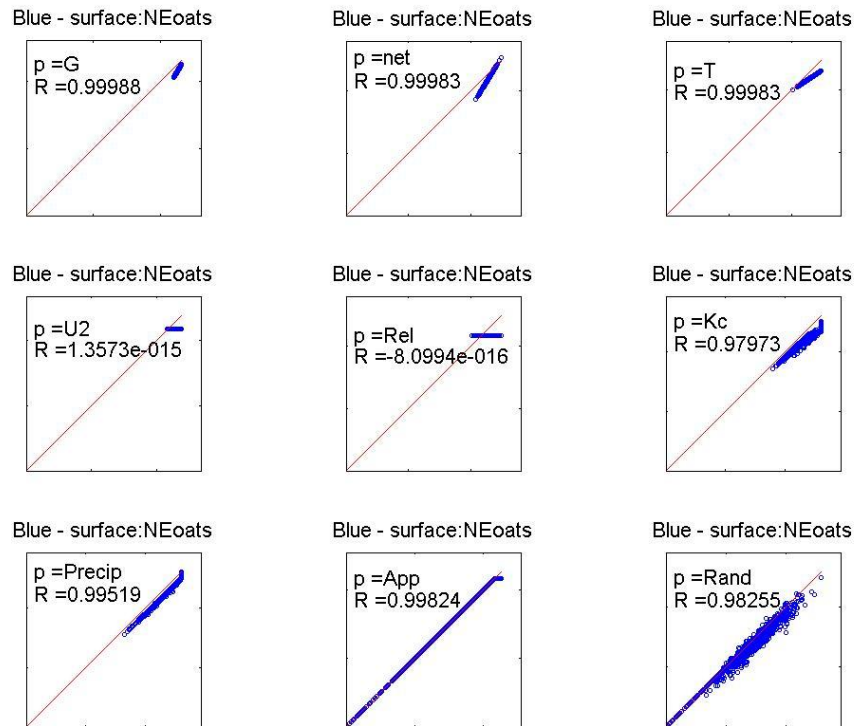


Figure 30: Scatter plots of surface water consumption for Nebraska oats, FAO 56 (x-axis) vs. Priestley - Taylor (y-axis)

Note that parametric sensitivity for both the FAO56 and Priestley – Taylor methods are skewed right (Figure 31 and Figure 32), above the expected value of the characterization factor. Outliers are generated in the scaling of the water consumption to the water application, to produce unit less characterization factors for blue water consumption.

Table 17: Average range of sensitivity for consumption of surface water

	FAO56	PT
ground	41.80%	39.12%
net rad	41.65%	39.44%
temp	42.55%	39.02%
wind	41.99%	38.44%
relative	42.07%	38.44%
crop k	48.63%	49.10%
precip	49.27%	49.48%
application	17.78%	17.44%
All	37.27%	40.25%

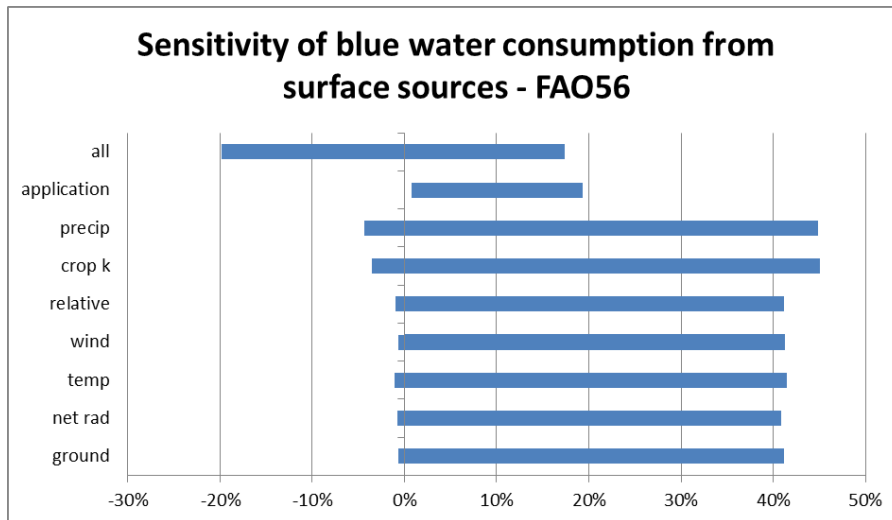


Figure 31: Average parametric sensitivity for surface water consumption, FAO56 method

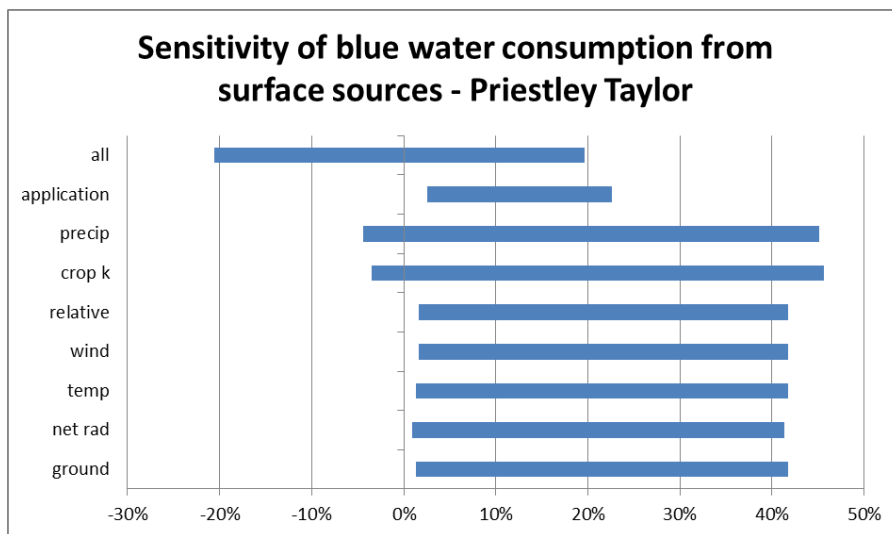


Figure 32: Average parametric sensitivity for surface water consumption, Priestley - Taylor method

Blue water consumption from ground water sources

Sensitivity to model selection

Ground water was applied as irrigation water for 29 of the state-crop variables. Twenty of those variables have a statistically significant difference between the FAO56 method and the Priestley-Taylor method. The following state-crop variables showed no statistically significant difference between models: Alabama cotton, Colorado spring

wheat, Georgia corn, Kansas corn, Louisiana cotton, Montana winter wheat, Texas corn, Washington spring wheat, and Washington winter wheat. These state-crop variables without a statistically significant difference between models are similar to surface water consumption for Nebraska spring wheat, in that the maximum water applied is very near or less than the minimum crop water deficit. Absolute differences between models for these state-crop variables range from 0% to 0.4% (Georgia corn). The cumulative results of spring wheat grown in Colorado are displayed in Figure 33; the highest value of groundwater application (dot-dash line) is below the lowest value of crop water deficit, thus climate parameters do not influence the characterization factor for this state-crop.

Of the 18 state-crop variables that exhibit statistically significant differences between the two models, the maximum average absolute difference was 18%, the minimum absolute difference was 0%, with an average of 4.3%. For individual state-crop variables, the variation of absolute difference for individual parameters ranges from a minimum of 0% for perfectly correlated estimates, to a maximum of 18% for Texas peanuts. Like surface water consumption, the sensitivity to model choice for ground water consumption estimates varies in magnitude across all state-crop variables.

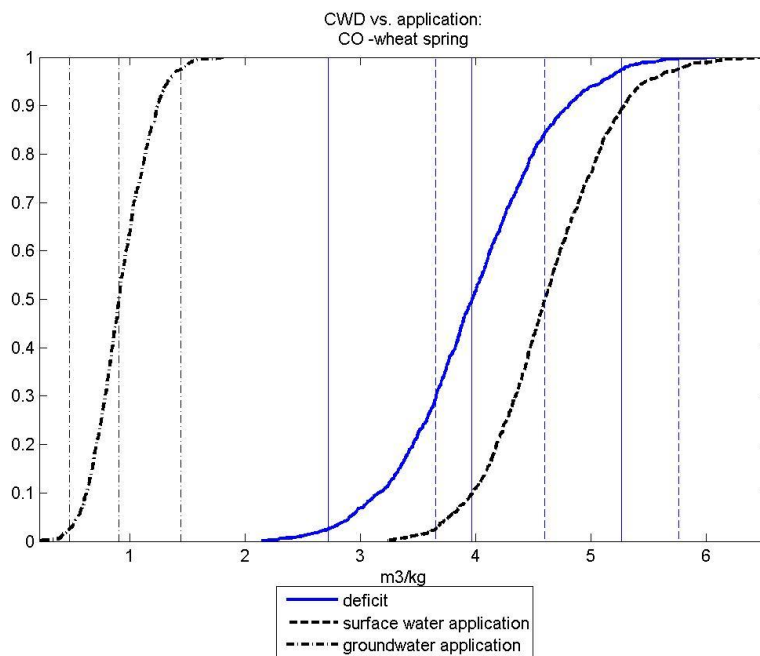


Figure 33: Cumulative results of crop water deficit and surface water application for spring wheat grown in Colorado– FAO56

Parametric Sensitivity

For groundwater consumption, parametric sensitivity was estimated using the same procedure used for surface and green water characterization. For the FAO 56 method, the average sensitivity ranges from 20% of the estimate for water application to 113% of the estimate for precipitation. For the Priestley – Taylor method, the average sensitivity ranges from 16% for water application to 110% for precipitation and crop coefficients. Average variation for the expected values of the FAO56 and Priestley – Taylor methods are 28% and 41% respectively (Table 18).

Table 18: Average range of sensitivity for groundwater consumption

range	FAO56	PT
ground	111.9%	110.5%
net rad	112.0%	110.9%
Temp	112.0%	110.4%
Wind	111.9%	110.1%
Relative	111.9%	110.1%
crop k	112.6%	113.6%
Precip	113.2%	113.9%
application	17.10%	17.73%
All	28.17%	34.34%

For groundwater consumption estimated by the FAO56 method, Texas corn is the most sensitive state-crop variable, with a variation of 900% for climate parameters. The next most sensitive is spring wheat grown in Washington state with a variation of 300% of the estimate for climate parameters. Estimates from the Priestley – Taylor method are similarly sensitive.

Normality

A χ^2 goodness-of-fit test is performed to determine if the estimates of characterization factors are described by a normal distribution. The MatLab function `chi2gof` was used for this work to perform the goodness of fit test. The χ^2 goodness-of-fit test (also known as the Pearson's chi-squared test) tests whether the frequency distribution described by a sample was produced from a normal distribution. `Chi2gof` calculates the summary statistics of the characterization factor samples, and then uses those statistics to produce a normal distribution of samples, by first aggregating the sample to a set of bins, and then calculating the χ^2 statistic on the frequency of occurrence in those

bins. The χ^2 test statistic is presented in Equation 33, where O_i is the observed frequency of bin i , and E_i is the expected frequency of bin i .

Of the 112 state-crop variables for green water consumption, chi2gof rejected the null hypothesis for 60, for both the FAO56 and Priestley – Taylor methods. That is, the samples for 60 state-crop variables do not fit a normal distribution at a 95% confidence interval. Chi2gof failed to reject the null hypothesis for 52 state-crop variables for which the normal distribution reasonably represents the green water characterization factor. For surface water consumption, chi2gof rejected 20 of the 54 state-crop variables modeled with the FAO56 method, and 21 state-crop variables modeled with Priestley-Taylor. Chi2gof failed to reject the FAO56 estimate of Washington spring wheat, but rejected the Priestley- Taylor estimate. For groundwater consumption, chi2gof rejected 28 of 29 state-crop variables modeled with the FAO56 method, and 20 out of 29 modeled with Priestley – Taylor. The FAO56 estimate of Idaho spring wheat was rejected, but chi2gof failed to reject the Priestley – Taylor estimates of the same state-crop variables. Conversely, chi2gof failed to reject the FAO56 estimate of Michigan corn, but rejected the Priestley – Taylor estimate

Equation 33: Chi-squared test statistic

$$\chi^2 = \sum_{i=1}^n \frac{(O_i - E_i)^2}{E_i}$$

3.3 Discussion

Green water consumption

The importance of characterization of green water variability is two-fold: the estimation of green water consumption impacts the estimation of crop water deficit and blue water consumption in turn, and changes in land-use change the amount of green water consumption within a watershed, affecting the local water cycle. Thus, neglecting the variability of green water consumption fails to address uncertainty in not just land use impacts, but also propagates to uncertainty in the estimate of blue water consumption.

It is shown that both the FAO56 method and the Priestley – Taylor method respond to variations in the two critical parameters; quantity of precipitation water available and crop growing season. Both models are well correlated across all parameters for all state-crop variables aside from wind speed and relative humidity, which contribute a

minimal amount of variability to the FAO56 method. However, the simpler Priestley – Taylor method underestimates the characterization factor for all state-crop variables. With the availability of time series approximations of wind speed and relative humidity publically available, the bias associated with the simpler model is not worth the slight reduction in computational complexity.

Perhaps one of the largest and as of yet un-characterized aspects of green water consumption is the impact of evapotranspiration on local precipitation due to atmospheric recycling (described in greater detail in 2.8).

Atmospheric recycling creates a feedback loop connecting land cover and land management to water availability.

Water consumed through evapotranspiration enters the atmosphere as water vapor, some of which may return to the originating basin as precipitation, and is therefore not considered consumption as defined by (Owens 2001). Thus, the variability of green water consumption characterization factors is important. Furthermore, this work finds a significant magnitude of variability for all state-crop variables, ranging from 16% to 50% of the estimate. This level of variability, and the associated uncertainty of atmospheric recycling, demonstrates need for caution when applying water consumption characterization factors for future land cover scenarios: a change in land cover will affect both the amount of soil moisture consumed, and the amount of precipitation available in a given watershed.

Blue water consumption

The larger ecological relevance of the variability in green water characterization factors is also applicable to the consumption of blue water. Some portion of irrigation water consumed may stay in the originating basin as recycled precipitation, thus the amount of water available is partially dependent on the amount of blue water consumed locally. Also, like the green water characterization factors, a large variation in blue water characterization factors was found for all state-crop variables. However, a high level of sensitivity to model choice was also found for blue water characterization from both surface and groundwater sources. The impact of model choice is dependent on the amount of application water and associated level of crop water deficit. A large difference between crop water deficit and water application tends to de-emphasize the importance of model selection, and thus variability in climate parameters. Irrigation water applied in quantities close to the amount of crop water deficit tends to compound the variability in both application data and climate data, generating larger levels of uncertainty and greater sensitivity to model selection. There are three general cases describing the interaction of individual parameters in the estimate of blue water characterization factors:

- Variability limited by the amount of water application
- Variability limited by the crop water deficit
- Variability compounded by both deficit estimation and water application.

Variability limited by the amount of water application is a case of a crop being produced under some amount of water stress. Under the given assumptions, all of the water available as soil moisture will be consumed as crop evapotranspiration, thus the variability of the characterization factor will be dependent entirely on the variability of water application. Under these conditions, the selection of characterization model is only relevant if the choice of model causes an overlap of deficit with water application. The cumulative results of the Monte Carlo sampling for surface water irrigation for Nebraska spring wheat is plotted in Figure 34 with crop water deficit estimated with the FAO56 method. Irrigation water from surface sources is plotted as the dashed line, and its 97.5 percentile is well below the 2.75th percentile of the crop water deficit. Thus, the 95% confidence interval for surface water consumption is determined almost exclusively by the variability in irrigation water application.

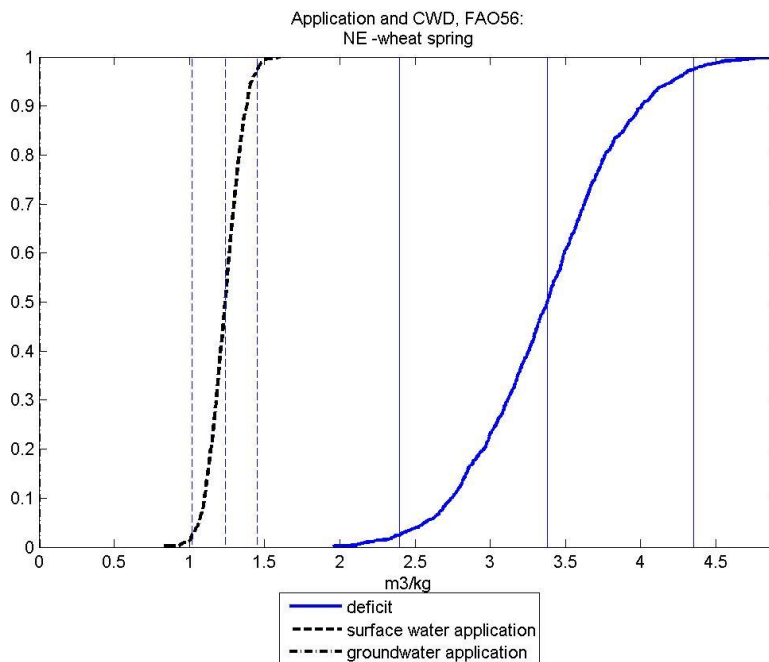


Figure 34: Cumulative results of CWD and water application for Nebraska spring wheat, FAO56 method

Variability limited by crop water deficit is the case where more water is applied than can be consumed by the environment. The crop is over-irrigated, and the variability of the characterization factor is entirely dependent on the estimate of crop water deficit. In this case, the choice of characterization model impacts the estimate of the characterization factor. The crop water deficit for Nebraska corn is plotted with irrigation from surface and groundwater sources in Figure 35. Surface water application far exceeds the level of crop water deficit, thus the variability in surface water application data does not contribute to the variability of the characterization factor.

Variability compounded by both crop water deficit and water application is the case where the amount of water application is close to the estimate of crop water deficit. Referring again to Figure 35, groundwater application, the dot/dash plot, is aligned with crop water deficit. Most of the 95% confidence interval of water application lies within two standard deviations of the crop water deficit. Thus, the characterization factor is sensitive to climate variability, model selection, and to water application. Subsequently, the variability of the groundwater characterization factor is larger than the estimate of the characterization factor itself.

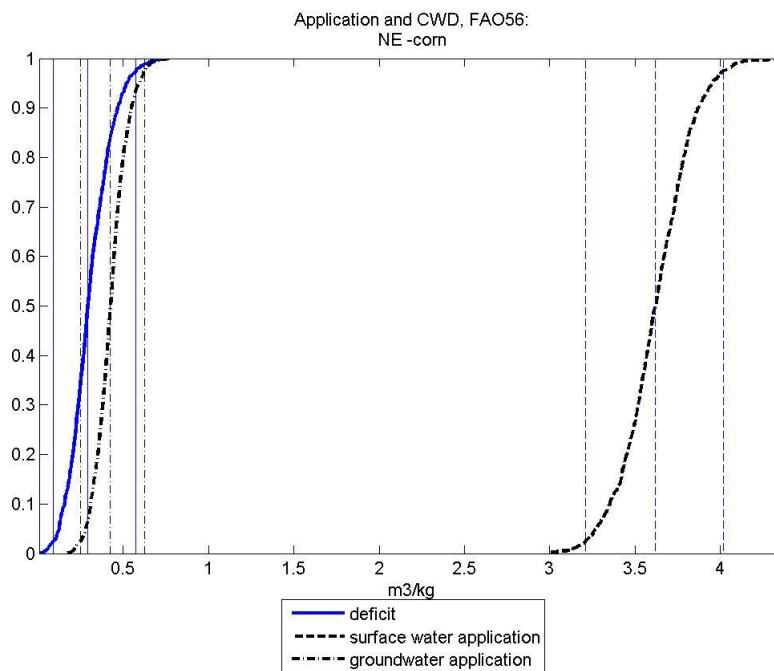


Figure 35: Cumulative results of CWD and water application for Nebraska corn, FAO56 method

Normality of characterization factors

There are several interesting insights into the probability distributions of water characterization factors. The Monte Carlo sampling generates a range of samples of characterization factors without performing the arithmetic of random variables. Although the individual climate parameters are random variables described by continuous probability distributions, several elements of the characterization models are piece-wise defined or otherwise non-continuous. Piece-wise defined elements of the characterization models include the estimation of effective precipitation, crop water deficit, and blue water consumption. Other non-continuous elements include truncated distributions for parameters bound to discrete intervals, such as depth of water application and precipitation (positive semi-definite) and shares of surface and ground water (ranging from $[0,1]$). For state-crop variables that fit within the continuous portion of the probability distributions describing the individual parameters, the subsequent characterization factors will fit a normal distribution, or be nearly normal. For those state-crop variables with characterization factors sampling from either component of a piece-wise defined function, the assumption of normality of the expected value is no longer reasonable. As such, a clue as to how the various components of the characterization model are interacting with each other can be gleaned from whether or not the results can be accurately described by a normal distribution.

Uncertainty in regions of water stress

The larger impact of a unit of water consumption depends upon the amount of water available in the locality of consumption, and the amount of demand on available resources. Several approaches have been developed to characterize the demand to availability ratio, known generally as water stress indices. The review paper of Brown and Matlock (2011) three general classes of indices:

- Indices based upon meeting basic human water requirements: such as per capita use versus availability regional availability.
- Human water requirements, including non-domestic uses such as industrial and agricultural production.
- Indices including environmental and ecological water requirements.

The common goal of all of these classes of approaches is to identify a level of sustainable water withdrawal for a particular region. These indices have been integrated into LCIA methodologies as a means to characterize the level of intensity of water use on a particular region; one unit of consumption in a high stress region will have a greater

impact than the same unit of consumption in a low stress region. Such water stress indices are employed as a second characterization model, scaling the impact of water consumption by the level of economic, ecological, and human dependence on the water resource. The development of water stress indices requires a complex harmonization of hydrological and economic modeling, and is beyond the scope of this dissertation.

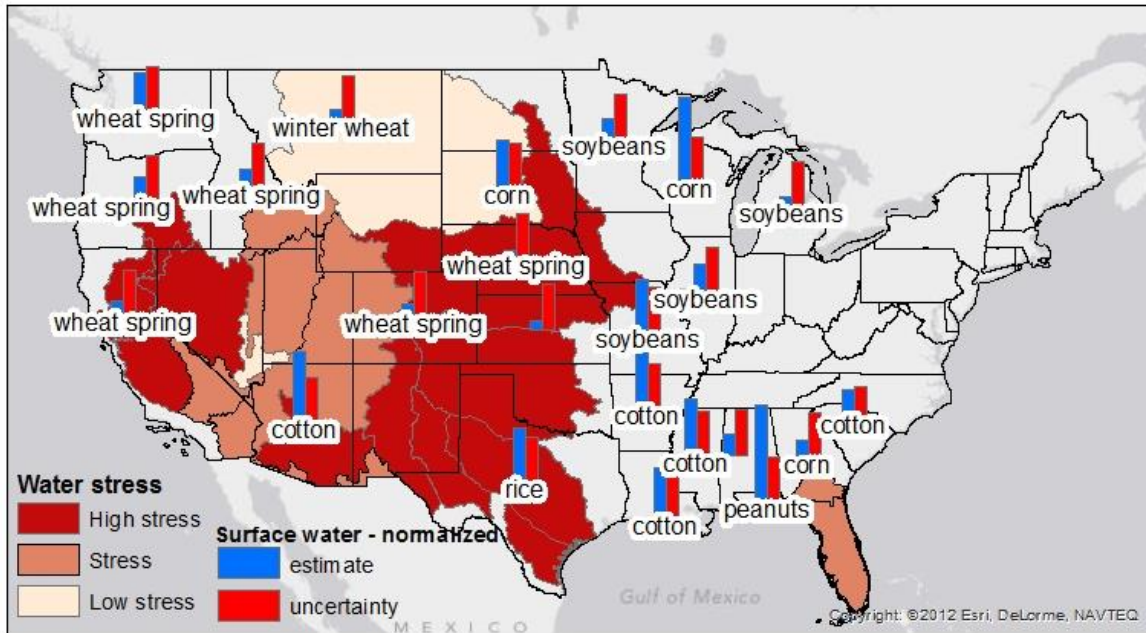
For illustrative purposes, the level of uncertainty and variability for freshwater characterization factors are superimposed on a regional map of US water stress. Water stress displayed here is from *The Atlas of Global Conservation* (J. Hoekstra et al. 2010), as a representation of the water stress index (WSI) for the continental United States at the scale of eco-region (See Section 2.7 and Section 2.8 for details).

As an example of the importance of characterizing uncertainty and variability of water consumption, the range of values of characterization factors is plotted over WSI levels from (J. Hoekstra et al. 2010). Four classes of water stress are represented in Figure 36 and Figure 37: no stress (white), low stress (light tan), stress (tan), and high stress (brown). The relative magnitude of water consumption characterization factors are represented by column graphs, the left column is a unit of water consumption (blue or green), and the right column is the relative magnitude of the combined uncertainty and variability (red).

Fifteen of the ARMS program states are under some level of water stress. Of these 16, 12 produce crops irrigated with water from surface sources, and 10 produce crops irrigated with groundwater. For crops irrigated from surface water sources, the following states are under a high level of water stress: Texas, Arizona, Colorado, Kansas, Nebraska, South Dakota, California, and Oregon. The following high stress states produce crops irrigated with groundwater: Oregon, Arizona, Kansas, Texas, California, Colorado, and Nebraska.

For those highly stressed states with irrigated agriculture, the magnitude of uncertainty of blue water consumption indicators can exceed the estimate themselves. For surface water consumption, spring wheat in Nebraska, Colorado, California, and Oregon all have a 95% confidence interval that exceeds the estimate itself. Groundwater consumption in highly stressed states is similarly variable for cotton grown in Arizona. Thus, the importance in quantifying the uncertainty and variability in characterization models is vital, for all steps of the LCIA.

Uncertainty of blue water consumption from surface sources



Uncertainty of blue water consumption from ground sources

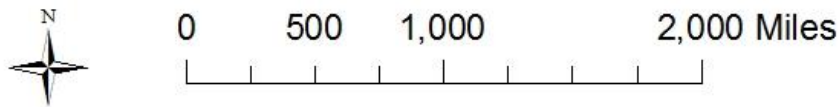
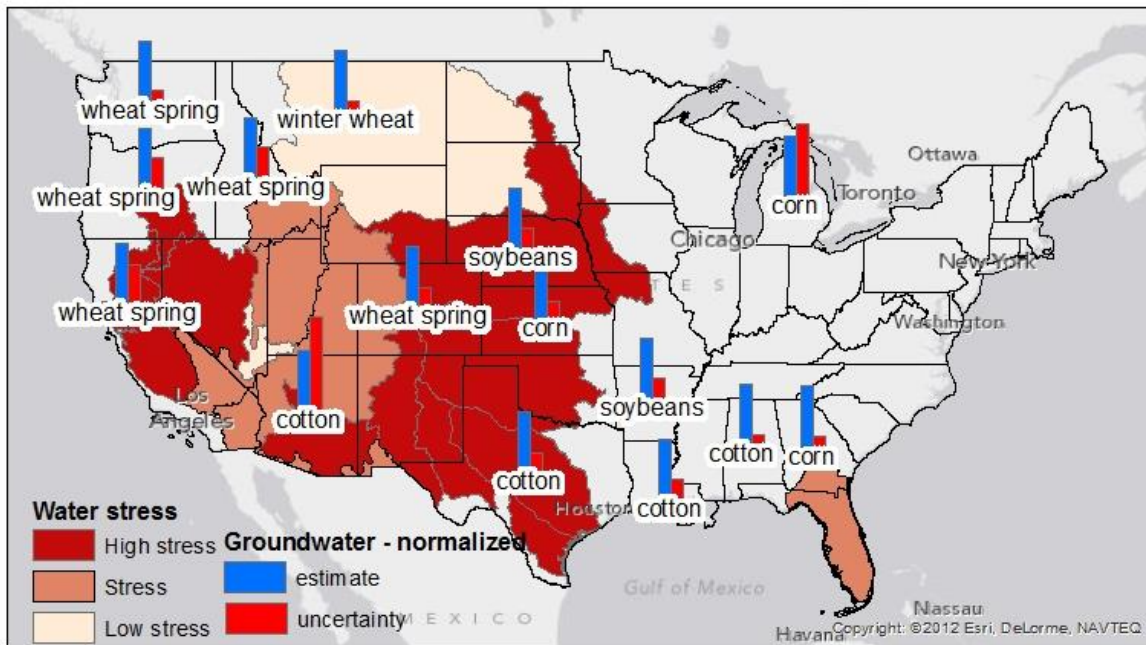


Figure 36: Blue water consumption and water stress of eco-regions

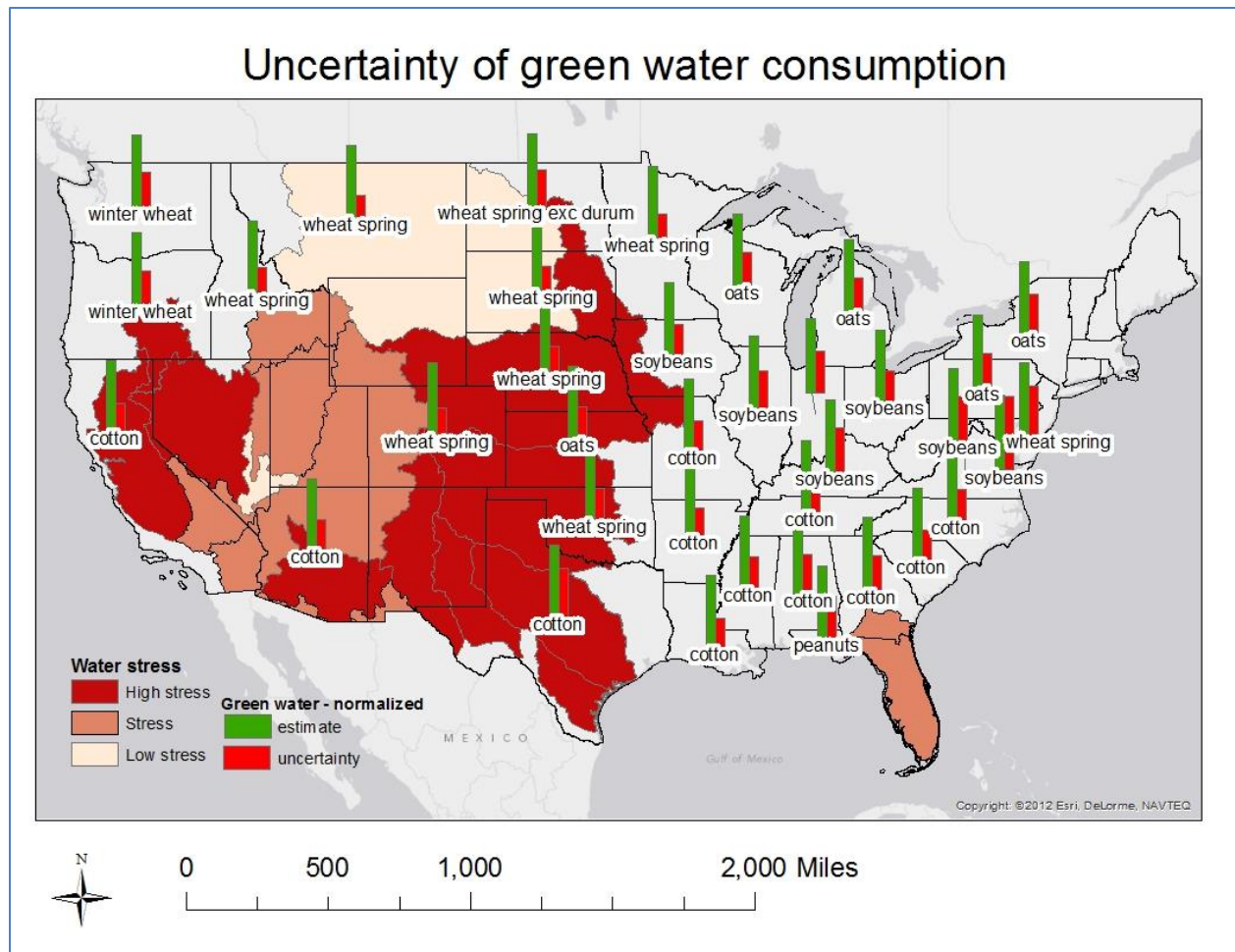


Figure 37: Green water consumption and water stress of eco-regions

Summary of approaches

The Hargreaves equation was studied in the preliminary sensitivity analysis as a simple regression model to be compared to the uncertainty associated with un-characterized parameters in the FAO 56 method. For the production of corn, the Hargreaves equation consistently produced characterization factors with a tighter range of estimates than the FAO 56 method. Whether the tighter range of estimates is representative of improved accuracy of the model, or oversight of important variability, could not be determined with the level of information used in the preliminary sensitivity analysis. As a regression formalization, and not a physical model, it cannot be asserted that the Hargreaves equation's reduced variation is representative of reduced uncertainty – the function of the regression is to minimize error between observations and model. Application of the Hargreaves equation is suited for estimating local reference evapotranspiration at short time scales for management purposes, such as irrigation planning of a

specific field when instrumentation for measurement of local relative humidity and wind speed is not available. For the development of characterization factors with robust representation of variability, the use of the Hargreaves equation is not recommended.

Characterization factors are well correlated between the FAO56 and the Priestley – Taylor methods for green water consumption, and for blue water consumption in either the CWD or the application limited cases. Although well correlated, the Priestley – Taylor method consistently underestimates characterization factors – this bias can be considered the uncertainty associated with using a reduced parameter model. Including estimates of climate parameters in the FAO56 method improves the representation of actual variability in the characterization factors, while simultaneously reducing the amount of uncertainty associated with a simpler model.

With the availability of gridded datasets for climate parameters, including estimates of relative humidity and wind speed, the case for using reduced parameter models for estimation of characterization factors weakens. When using widely available data, such as the climate inputs for the VIC model used here (Maurer et al. 2012) the increased computational complexity of implementing the FAO56 method is minimal. Thus, the FAO 56 method is recommended for the development of LCIA characterization factors, due to its reduction of uncertainty, and improved representation of variability compared to reduced parameter approaches.

3.4 Conclusions

Significant ranges in results for green water consumption due to climate variability were found, irrespective of the modeling approach used. Impacts to the water cycle due to land cover and land use changes are poorly described in the current LCIA approaches and the wide range of reasonable values for green water consumption must be considered in uncertainty analysis for comparative assessments.

A significant range in results for blue water consumption was also found, and the nature of the range of results depends on the level of irrigation taking place at the farm. The importance of model selection enters into the results only in cases when irrigation application is equal to or greater than the crop water deficit. For areas where the crop is under-irrigated, the model selection does not enter into the results. In the case when irrigation is nearly equal to the crop water deficit, the climate variability compounds with the irrigation application uncertainty, and can produce large ranges of impact factors. When making comparative assertions, the inclusion of parametric variability as well

as model uncertainty must be included. With the availability of gridded datasets, the implementation of the FAO56 method is straightforward, and the use of simpler models, and reduced datasets such as CLIMWAT, are neither necessary nor recommended.

4 Assessing Freshwater Consumption in LCA at the Regional Level

There is a substantial body of work on mapping the origin and fate of atmospheric water vapor at a range of spatial scales, and a number of issues persist at this time (see (Trenberth et al. 2007) and (Van der Ent et al. 2010) for examples). Variability associated with temporal and spatial scales and with boundary selection has a substantial impact on the magnitude of the water footprint. Uncertainty associated with data consistence and availability also contributes to the range of possible values for water footprinting. An in-depth analysis of the contribution of variation and uncertainty of atmospheric recycling on water footprints is beyond the scope of this study. Presented here is an exposition of the impact of atmospheric recycling on water footprints based on work in the literature.

4.1 Variability: spatial scale of control volume

As noted above, the spatial scale of the control volume directly affects the recycling ratio, and therefore the overall impact of water consumption on resource scarcity and other associated impacts. Trenberth estimates the impact of the length of the control volume on the magnitude of the recycling ratio (Trenberth 1999). In order to demonstrate the effects of length scale on the recycling ratio, Trenberth presents the simplified, 1-dimensional atmospheric water balance as a function of length (Equation 34). A simplifying assumption is that the total change in atmospheric water vapor is the average of the incoming and outgoing water (Equation 35). Assuming that the air column is well mixed, and that the total change in atmospheric moisture storage is negligible, the recycling ratio from Equation 12 can be rearranged as a function of length, evaporation, and precipitation (Equation 36). For this simplified model, Trenberth shows that the recycling ratio is highly dependent on the length scale of the control volume. For example, for a length scale increase from 100 km to 1000 km, the recycling ratio can increase an order of magnitude, from 2% to 25%, for a fixed atmospheric flux and evaporation rate. Recycling ratios as a function of length scale and atmospheric flux are plotted for a fixed evaporation rate ($5 \cdot 10^{-5} \text{ kg/m}^2 \text{ s}$) in Figure 38, using Trenberth's length function (Equation 36). For a fixed evaporation rate, increased moisture advection corresponds to a lower recycling ratio. Similarly, as the length scale increases, the recycling ratio increases for the same rate of moisture flux.

Equation 34: 1-dimensional water balance, as described by (Trenberth 1999) where $F_{out} - F_{in}$ is the moisture flux, E is the evapotranspiration, P is the precipitation, and L is the length scale of the control volume.

$$F_{out} - F_{in} = (E - P)L$$

Equation 35: Average moisture flux

$$F = 0.5 * (F_{out} + F_{in})$$

Equation 36: Recycling ratio as a function of evaporation (E), precipitation (P), length (L), and incoming moisture flux (F_{in})

$$\rho = \frac{EL}{EL + 2F_{in}}$$

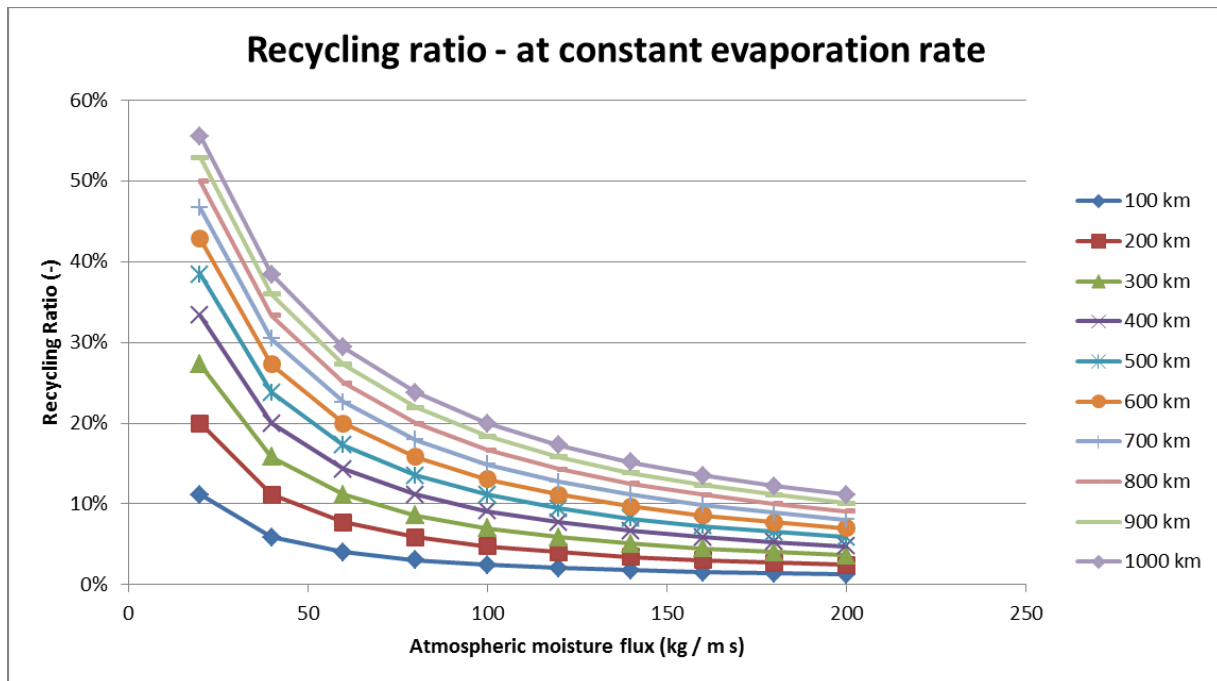


Figure 38: Moisture recycling for a range of length scales ($E = 5e-5$ kg / m² s)

4.2 Variability: changes over time for agricultural production

As a climate driven phenomenon, atmospheric water recycling varies over time and over a range of time scales.

Typical time-steps for agricultural crop production studies are day, month (as used in this dissertation), or growing season. Van der Ent et al. estimated continental water vapor recycling at a 1.5 x 1.5 degree grid, using 10 years of

data at the 3 hour time step (Van der Ent et al. 2010). The difference in average recycling ratios between January and July ranges from 0 – 40% for the West Coast, to 10 – 80% for the Mississippi Basin. Dominguez et al. present continental US recycling ratios for monthly time-steps over a 1×10^6 km² grid (Dominguez et al. 2006). Variation in recycling ratios in Northern climates ranges a few percentage points over the course of June, July, and August. Recycling ratios over the same period can vary by $\pm 10\%$ of the average in southern regions such the Southwest or the Mississippi delta. Dominguez et al. also consider the evaporation ratio, or the amount of precipitation that originated as evaporation from elsewhere on the continent. For the Western United States, the difference in average evaporation ratios ranges from 40 – 70%, and ranges from 20 – 40% for the Mississippi basin.

Dominguez et al. also perform an empirical orthogonal function (EOF)²⁷ analysis on the data, and identify spikes and variations over time, in specific regions. In the western and southwestern US, annual recycling ratios can vary $\pm 10\%$ of the average, using data from 1979 to 2000.

4.3 Data uncertainty

Given the variability of time and space, use of a consistent climate dataset for calculating the mass balance is of great importance. However, in their analysis of variability in modeling atmospheric water vapor, Trenberth et al. note that currently available atmospheric datasets do not close the mass balance. The climactic data used for estimating atmospheric water vapor are based on point observations and satellite data, which are then statistically reanalyzed to produce continuous grids of information. Errors are produced in both the measurement of the data, and in both spatial and temporal gaps. These data gaps represent uncertainty in the estimation of atmospheric water vapor, and the subsequent estimates of recycling.

Dominguez et al. explicitly address the issue of data gaps and uncertainty by including a residual term in their atmospheric water balance equation. A sub-daily time keeps track of the change in water storage term (Dominguez et al. 2006) and the residual term measures the size of the data gap corresponding to the amount of water vapor missing from the atmospheric water mass balance. Dominguez et al. find, for the continental United States, the size of the residual is within an order of magnitude of the advection term, and roughly 10% of the evapotranspiration and precipitation terms for both daily and monthly time scales (Table 19). Noting the residual represents systematic

²⁷ An empirical orthogonal function analysis is a decomposition of a set of data into a set of orthogonal basis functions, conceptually similar to an eigenvalue decomposition of a single function.

error (as opposed to a random error), the authors were unable to establish how much of the error is associated with the individual parameters in the water balance²⁸.

Equation 37: Atmospheric water balance, with residual term α (Dominguez et al. 2006)

$$\frac{\delta f}{\delta t} + \nabla * f * \bar{v} = E - P + \alpha \text{ (units of } L/T)$$

Table 19: Average values for parameters in Equation 37 for Continental US from 1979 - 2000 from (Dominguez et al. 2006)

Parameter	Monthly	Daily
α	-0.34	-0.10
$\delta f / \delta t$	-.00	-0.00
$\nabla * f * \bar{v}$	0.06	-0.08
E	3.00	3.05
P	2.36	2.60

4.4 Discussion

In summary, the physical mechanisms driving water scarcity impacts operate on multiple time and length scales (time ranging from the day to the year and for length ranging from the farm level to the basin level scale).

Furthermore, there is a coupling between green water consumption and blue water consumption all scales. At the farm scale, the level of green water consumption determines the potential for blue water consumption. At the basin scale, changes in land cover produce changes in green water consumption, which impact both the amount of irrigation water needed to produce high yield crops, and the amount of water available. That is, land cover impacts both the numerator and denominator of the water stress index (see section 2.7 and Equation 38).

Equation 38: One form of the WSI, restated from section 2.7. Represented as the sum of domestic, industrial, and agricultural uses (D, I, and A respectively), divided by the sum of all discharges (Q)

$$WSI = \frac{\sum D + I + A}{\sum Q}$$

Based on the literature, a bound can be placed on the impact the neglect of atmospheric recycling plays on water consumption estimates. Consider the regional level water consumption estimated as the total of the local consumption including local recycling, minus the sum of consumption due to recycled precipitation from outside the

²⁸ See also (Trenberth, Fasullo, and Smith 2005) for further discussion of uncertainty in atmospheric water vapor.

control volume and consumption due to recycled precipitation that leaves the control volume. Considering just green water, a simple adjustment for regional consumption can be done by Equation 39. The uncertainty propagates through Equation 39 linearly, thus the interval arithmetic is dominated by the parameter with the largest uncertainty. Ranges of uncertainty are summarized in Table 20.

Equation 39: Adjustment of green water consumption, accounting for atmospheric recycling. GW_r is regional green water consumption, GW_l is local green water consumption, ρ is recycle ratio, ε_i is the evaporation ratio of the originating basin, ε_o is the evaporation ratio of basin receiving recycled water from original basin, and $GW_{p,o}$ and $GW_{p,i}$ are the components of green water consumption due to recycled precipitation for the originating basin and other basins, respectively.

$$GW_r = GW_l * (1 - \rho) - GW_{p,o} * \varepsilon_i - GW_{p,i} * \varepsilon_o$$

Table 20: Uncertainty associated with scaling farm level consumption to the regional level, in the US.

Recycling ratio (% water consumed)	Minimum	Maximum
Region	0.1	0.8
Length scale	0.0	0.5
Temporal scale – seasonal	0.0	0.8
Temporal scale – annual	0.0	0.1
Data gaps	0.0	0.1

Water consumption at the farm level should be considered a conservative estimate—at that length scale the recycling ratio is effectively zero. At spatial scales greater than the farm, over temporal scales longer than a day, atmospheric recycling serves to reduce the overall impact of freshwater consumption. However, to integrate atmospheric recycling into water consumption indicators, the following questions must be addressed:

- At what spatial scales should water consumption be considered?
- What is an appropriate time-step to evaluate water consumption, so as to capture the effects of atmospheric recycling?
- How can the recycling of evaporated water from a product be verified?

As defined by Owens's, the availability of consumed water in its originating basin determines whether the water has been consumed. However, in the context of LCIA there has as of yet not been a determination of what qualifies as a

basin. Evaporated water from one area may precipitate over another region within the catchment of the same major river. While downstream users may not notice the full impact of local water use because of the atmospheric recycling, to upstream users or those along other tributaries the regional impact is on the order of the farm level impact. In addition to choosing an appropriate spatial scale, developing an understanding of the transit of atmospheric water vapor as a network is necessary to determine how much the evaporated water from one region contributes to the precipitation of another.

As Berger and Finkbeiner note, each stage of impact characterization involves the modeling of complex interactions between the surface and the atmosphere, at a range of spatial and temporal scales, and critical consideration of regional atmospheric recycling has presently been neglected (Berger and Finkbeiner 2012). Furthermore, the authors note that the uncertainty associated with all of the characterization models employed, and the trends and variability of the independent parameters, have not been assessed. It is proposed that these uncertainties are substantial, and until they are characterized, water footprints do not meet the standards outlined in ISO 14044.

5 Beyond Water Stress: investigating the water – energy nexus

Both water and energy are critical elements of sustaining life. At the subsistence level, freshwater is an essential requirement for health, hygiene, food production and preparation, and maintenance of critical ecosystem services. Similarly, at the level of life support energy is essential for heating and food preparation. Beyond subsistence, the improved quality of life enjoyed by many is possible because of access and development of water and energy sources. These benefits include consistent access to healthy and affordable food, affordable transportation over increasing distances, improved communication, and the increase in life-span and quality from better medicine and technology. In as much as water and energy are independently critical to society, the production and maintenance of water and energy resources are highly interdependent. Water is required to produce energy, and energy is required to access water. This interdependence is commonly known as the Water-Energy Nexus, and in regions of resource scarcity this complex network can create conflict between competing interests and stakeholders.

Water and energy interconnectedness is reviewed in the survey by Gleick (Gleick 1994). Energy is used to access water in a number of ways, particularly to overcome what Gleick describes as a gross “uneven spatial and temporal distribution”. Large amounts of energy are used to move water from points of access to areas of scarcity and high

demand. An extreme example is the California Water Project, which moves water from the San Francisco Delta to Southern California, pumping water up 2,000 feet of elevation at the Tehachapi mountains, at an energetic cost of 5 million MWh/yr (amounting to 2 – 3% of the total energy use in California) (Cohen, Nelson, and Wolff 2004).

Groundwater pumping and water desalination are other energy intensive water production activities, and the willingness to pay the energetic cost for water procurement increases in regions of water scarcity.

In as many ways as energy is critical to producing water, water is a critical component of energy production. It is fundamental as the working fluid in thermoelectric generation, which is the single largest user of water resources in the United States (Kenny et al. 2009), and hydroelectric generation. It is used in coal mining, oil and gas extraction, and indirectly in the production of solar and wind generation technology (Gleick 1994), and biofuel feedstocks (Chiu, Walseth, and Suh 2009).

A range of users often coexist within a single watershed, and water resources are shared among a range of competing users. Dams are employed to provide a reservoir for hydroelectric projects, as well as regulating stream flow and water access to upstream users, such as large scale irrigation projects. Power utilities managing hydroelectric facilities are often required by law to produce a minimum amount of power, maintain a minimum stream flow for ecological purposes, as well as provided water for irrigation projects. In times of water scarcity, these competing users can create conflict²⁹, particularly with changes in water flow and availability from the impacts due to climate change (Hamlet et al. 2010).

As is noted in previous sections of this dissertation, impacts to freshwater resources in the production of agricultural and bioproduct feedstocks are becoming a topic of interest in the systems and impact analysis communities.

However, in the context of the water-energy nexus, changes in water use and water consumption for agricultural production may indirectly impact energy consumption. Energy used in the application of irrigation water for agricultural production is estimated in the following sections.

5.1 Estimation of energy requirements for irrigation application

Irrigation processes used in the farm level crop production data in the LCA Digital Commons are classified by source and irrigation technology (see Chapter 3). Irrigation water is withdrawn from surface, ground, or unspecified

²⁹ For example, see the Clark Fork River Basin Management Plan, in Montana http://dnrc.mt.gov/wrd/water_mgmt/clarkforkbasin_taskforce/water_mgmt_plan.asp

water sources and is applied with pressure, gravity, or unspecified irrigation technology types. An irrigation unit process at the crop production level will include both the withdrawal and application sub –process, and has the form: *irrigate, <application type>, <source type>, in <year>, at farm.*

Energy for irrigation is divided into two sub-processes: energy used to abstract water from a source, and energy used to apply water to the field. To estimate the amount of energy required for each of these sub-processes, the total dynamic head is estimated. Head is the common term for the amount of potential energy associated with a column of water, and thus is measured in feet. Total dynamic head (TDH) expands the concept of head to all of the energy sinks in an irrigation system. A single crop production unit process can include several permutations of application technology and water source. For example, crop irrigation can include the following example flows:

- *irrigate, pressure, groundwater source, in 2000, at farm*
- *irrigate, gravity, groundwater source, in 2000, at farm*

Total dynamic head is calculated as the sum of four components: energy used for lift, pressure head, velocity head, and pipe losses (Equation 40). For each state, the estimates for application and withdrawal are calculated separately, and then combined (Equation 41). The amount of energy per unit of volume moved can be calculated by multiplying the total dynamic head by the density of water and the acceleration due to gravity (Equation 42).

Energy is then multiplied by a fuel specific plant efficiency to determine a unit of energy of fuel.

Equation 40: Total dynamic head (TDH) L , P , V , and μ are lift, pressure head, velocity head, and pipe losses respectively.

$$TDH = L + P + V + \mu \text{ (units of } L\text{)}$$

Equation 41: System head (TDH_{total}) as the sum of withdrawal (TDH_w) and application (TDH_a) head

$$TDH_{total} = TDH_w + TDH_a$$

Equation 42: Energy per unit of water applied, where γ , and g are the density of water and the acceleration due to gravity respectively, and α is a conversion factor

$$\frac{E}{vol} = TDH * \alpha * \gamma * g \text{ (units of } E / L^3\text{)}$$

Individual components of total dynamic head are estimated as follows. Lift is simply the vertical distance water is moved. For water withdrawal, this is the depth-to-water for a source. For water application, this is the height water

is elevated before application, such as with an overhead sprinkler system. Pressure and velocity head are estimated by normalizing the system pressure and system water velocity by the inertial component of water. System pressure is dependent on the type of irrigation system used (see Table 21), Pipe velocity is assumed to be an average of 5 ft/sec, which is the recommend velocity to avoid water hammer (Fips). Pipe losses are estimated using the Hazen-Williams equation³⁰ for pipe losses, which is an empirical formulation for estimating head losses (Equation 43).

Equation 43: Hazen-Williams equation for pipe losses, where c is a roughness coefficient, q is the flow rate, and d_h is the hydraulic diameter

$$f = 0.2083 * \left(\frac{100}{c}\right)^{1.852} * \frac{q^{1.852}}{d_h^{4.8655}} \text{ (units of } ft)$$

Data for estimating TDH comes from the Farm and Ranch Irrigation Survey (FRIS), a special supplement to the USDA Census of Agriculture, performed by the National Agricultural Statistics Service (National Agricultural Statistics Service). It has been included in the Census of Agriculture for the past four editions: 1992, 1997, 2002, and 2007. Data from the FRIS includes the number of acres irrigated by application technology type, acres irrigated by pumps of various fuel types, as well as the lift, operating pressure, and flow rates of irrigation systems.

³⁰ http://www.engineeringtoolbox.com/hazen-williams-water-d_797.html

Table 21: Application and energy technology types from the Farm and Ranch Irrigation Survey

Pressure Systems	Gravity Systems	Energy types
Center pivot, Low pressure, under 30 psi	Above ground pipe (except poly tubing)	Diesel
Center pivot, Medium pressure, 30 to 59 psi	Poly tubing (or other single year use, lay flat tubing)	Gasoline
Center pivot, High pressure, 60 psi or more	Open surface ditches lined	Liquefied petroleum gas
Linear move tower sprinklers, Low pressure, under 30 psi	Open surface ditches unlined	Compressed natural gas
Linear move tower sprinklers, Medium to high pressure, 30 psi or more	Underground pipe	Electricity
Solid set and permanent sprinklers, Low pressure, under 30 psi		
Solid set and permanent sprinklers, Medium to high pressure, 30 psi or more		
Side roll, wheel move, or other mechanical move		
Big gun or traveler		
Hand move		

Within pressure and gravity systems, the technology mixes are developed using the above FRIS data. The fraction of each type of application and energy to the irrigation process is estimated by dividing the area irrigated using each technology by the sum of all areas. For pressure irrigation, individual irrigation technologies are aggregated to low, medium, and high pressure systems. Energy requirements are estimated for systems operating at less than 30 psi, between 30 and 60 psi, and above 60 psi Table 22.

Table 22: Pressure irrigation system aggregation

Pressure Systems	Aggregated system type
Center pivot, Low pressure, under 30 psi	low pressure
Center pivot, Medium pressure, 30 to 59 psi	medium pressure
Center pivot, High pressure, 60 psi or more	high pressure
Linear move tower sprinklers, Low pressure, under 30 psi	low pressure
Linear move tower sprinklers, Medium to high pressure, 30 psi or more	medium pressure
Solid set and permanent sprinklers, Low pressure, under 30 psi	low pressure
Solid set and permanent sprinklers, Medium to high pressure, 30 psi or more	medium pressure
Side roll, wheel move, or other mechanical move	medium pressure
Big gun or traveler	high pressure
Hand move	high pressure

Uncertainty is estimated for each parameter in the estimate of energy usage. The FRIS includes RSE values for system pressure, flow rate, depth to water, number of acres irrigated by pressure and gravity technology types, and the number of pumps used in irrigation. Uncertainty associated with other parameters was subjectively modeled as either uniform or triangular distributions. A uniform distribution was applied when only an interval of possible expected values was available. A triangular distribution was used when the bounds of the interval of possible expected values were unlikely to occur. The following table summarizes the uncertainty information used in this study (Table 23). For the LCA Digital Commons, the uncertainty of individual parameters is not propagated to results until the estimation of the LCI—the unit processes are described by a set of parametric equations with associated uncertainty and probability distributions. When performing an LCA, the uncertainty is propagated to the LCI by either Taylor expansion or Monte Carlo estimation (see (Ciroth, Fleischer, and Steinbach 2004) for further description of uncertainty propagation in LCA). Here, independent parameters described by triangular or uniform distributions are propagated by Monte Carlo estimation with a 1000 replication sample size (yielding normal distributions for the dependent variables). Uncertainty is then propagated through to an energy inventory using a Taylor expansion approximation (see Equation 29)

Table 23: Parameters for estimating energy use for irrigation application

Parameter	Units	Distribution
Hazen-Williams pipe friction coefficient	-	uniform
plant efficiency	-	uniform
pipe velocity	ft/s	triangular
hydraulic diameter	in	uniform
pipe length	ft	triangular
system pressure	psi	uniform
energy type	acres	normal
application type	acres	normal
lift	feet	normal
pressure	psi	normal

5.2 Results

The amount of energy required to withdraw and apply water is displayed in Figure 39 for gravity and pressure irrigation systems, using surface and groundwater sources. Error bars in the graph represent the 95% confidence interval, or 1.96 standard errors above and below the average value. Arizona is the most energy intensive irrigator of the ARMS program states. Of the irrigation flows studied, pressure irrigation from groundwater sources is the most energy intensive ranging from 181 - 394 GJ/ha-m (Missouri and Arizona respectively). Gravity irrigation from groundwater sources is the second most energy intensive process, ranging from 76 – 288 GJ/ha-m of water applied (again for Missouri and Arizona respectively)

For nine of the ARMS program states, energy for gravity irrigation from groundwater sources exceeds pressure irrigation from groundwater sources. These states are Delaware, Illinois, Indiana, Maryland, Mississippi, Missouri, North Carolina, and North and South Dakota. However, with the exception of Missouri, the difference in average

values between gravity and pressure irrigation is statistically insignificant. In Missouri, irrigation of surface water is much more intense than for groundwater. For the program crops included in this study, irrigation water from groundwater sources is not applied in Missouri, suggesting that groundwater extraction surveyed in the FRIS represents small scale operations, relative to those withdrawing surface water (see Figure 40, rice grown in Missouri as an example).

Uncertainty is also greatest for the states with the highest energy intensity. Montana has the highest level of uncertainty, with an RSE value of 43.4% for gravity irrigation from groundwater sources. Other states with large levels of uncertainty include Arizona (RSE = 39.5% for gravity irrigation from groundwater sources), and Virginia (RSE = 41.3% for gravity irrigation from ground water sources).

The states with the lowest energy intensity also have the lowest associated uncertainty. Louisiana has the lowest energy intensity of all the program states, with 44 GJ / ha-m used to irrigate cotton with gravity fed surface water (the majority of water used to irrigate cotton in Louisiana Figure 41). The RSE associated with gravity irrigation of surface water for Louisiana is 5% of the estimate. Other states with low energy intensity irrigation include Arkansas (78.3 GJ/ha-m for gravity irrigation of surface water), and Florida (75.5 GJ/ha-m for gravity irrigation of surface water). These two processes have RSEs of 5.71% and 6.3% of the estimates respectively.

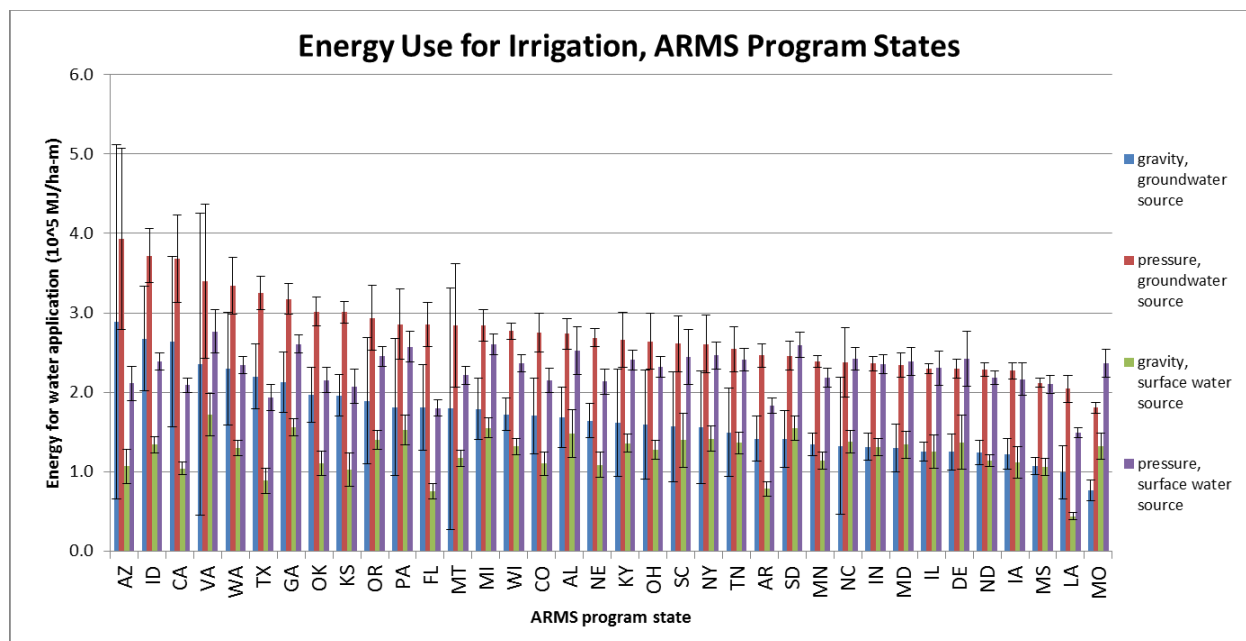


Figure 39: Energy use for irrigation application, ARMS program states

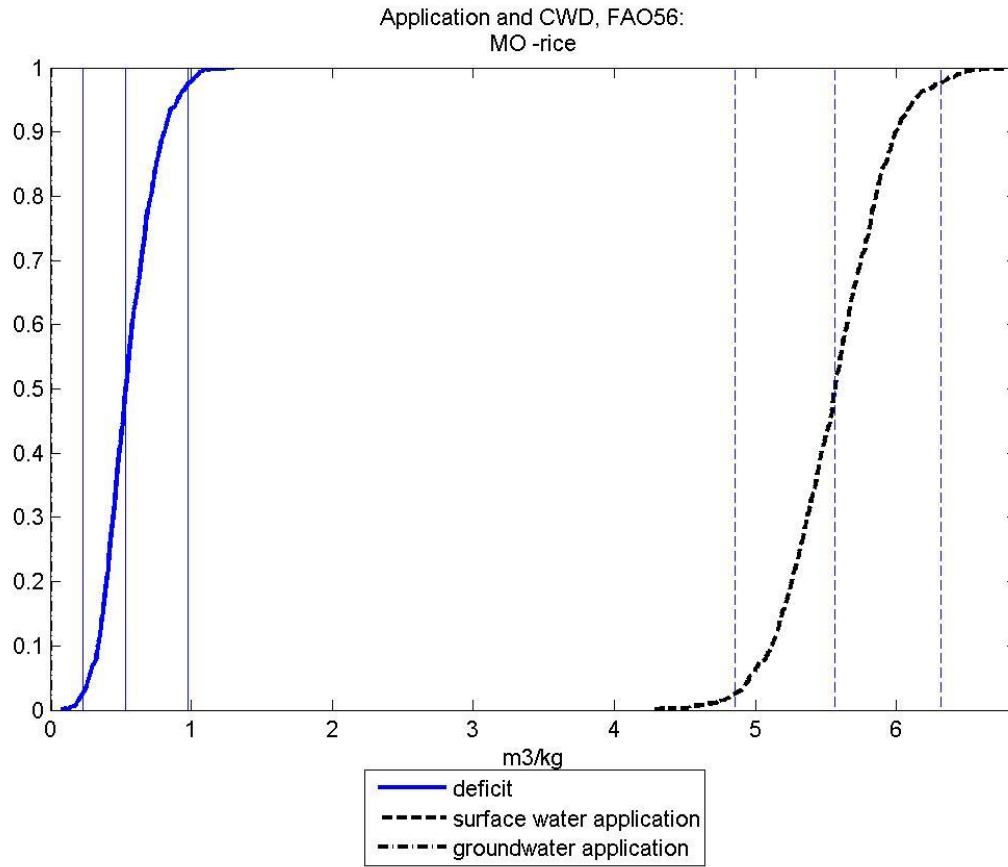


Figure 40: Freshwater application and crop water deficit for rice grown in Missouri, (note only surface water application included)

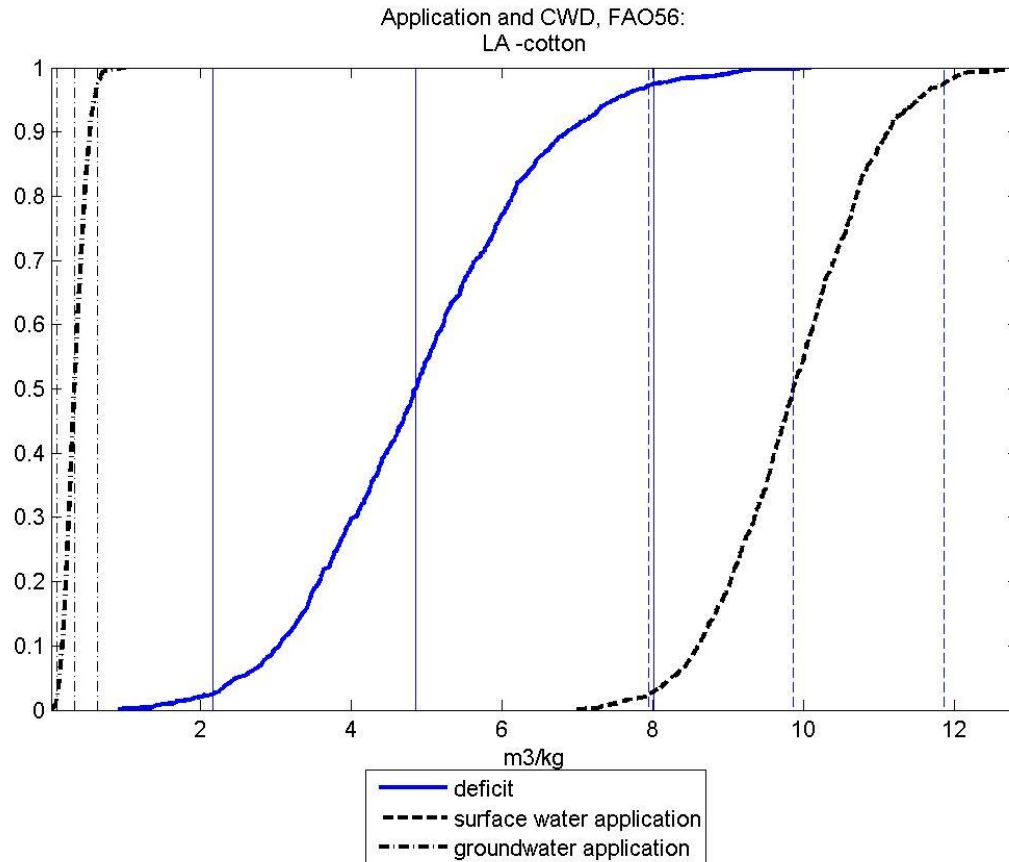


Figure 41: Freshwater application and crop water deficit for Cotton grown in Louisiana

5.3 Discussion

Referring again to Figure 39, irrigation using groundwater is the most energy intensive water application process. States experiencing some level of water stress in particular have a higher level of energy use for groundwater extraction than states not experiencing water stress (see Figure 42). These states include Arizona, Texas, and California. As water stress in these areas increases, more expensive is given to exploiting groundwater sources. In comparing the energy use of states experiencing some level of water stress to states not in a condition of water stress it is found that states in the Mississippi basin and the Great Lakes region (regions with plenty of access to surface water) use much less energy withdrawing and applying groundwater than southwestern states.

Further, water resources in some Western states (e.g. Arizona, Texas, and California) are governed by the prior appropriation doctrine. In prior appropriation states the first user in time has the first rights to water use. That is, the user with the earliest documented continuous productive use of a water resource has priority on that resource.

Because water rights are applied only to surface water resources, in states approaching full appropriation junior users seek other sources of water, including groundwater. Thus, because groundwater extraction is more energy intensive than surface water withdrawal, there is a possibility that water consumption impacts can be linked to increases in energy use at the water-energy nexus.

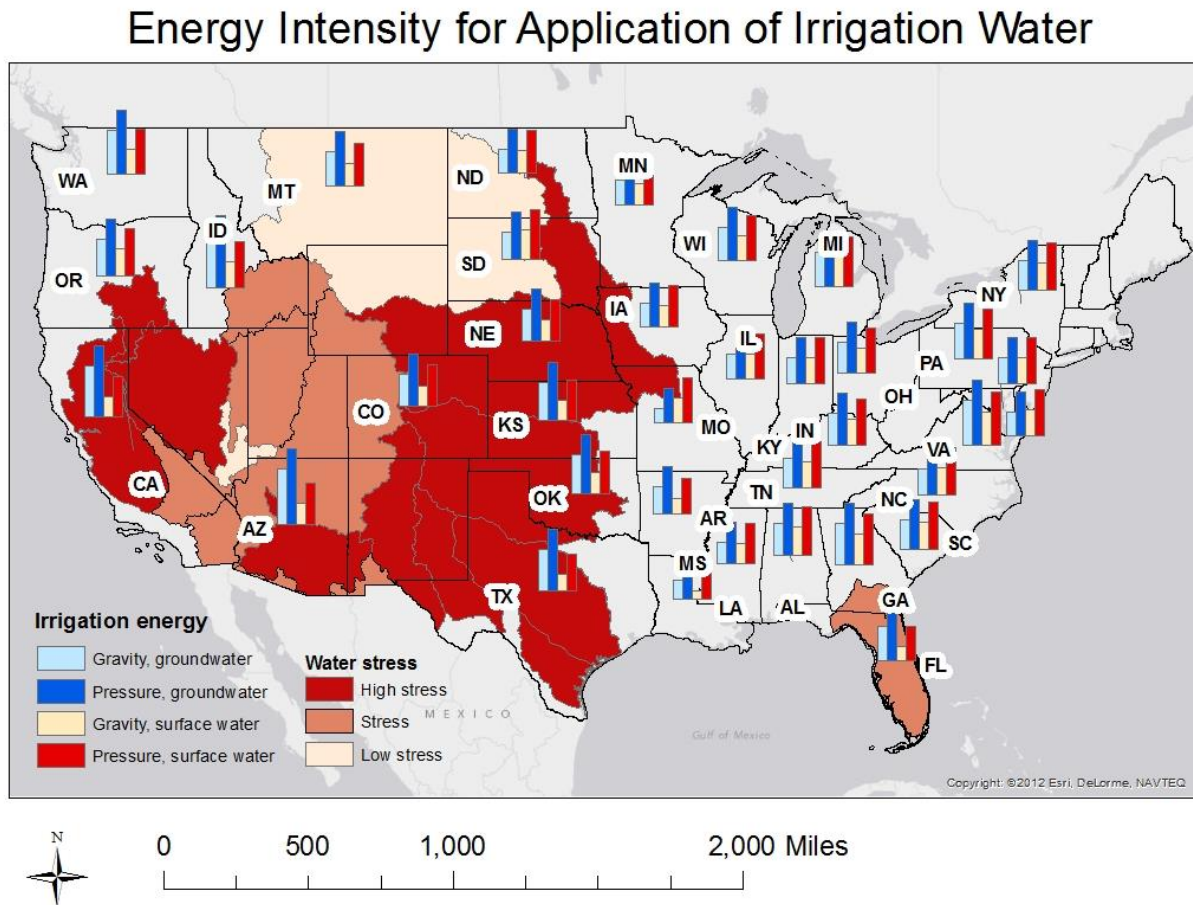


Figure 42: Energy intensity for application of irrigation water, for ARMS program states

To explore the situation further, consider for example cotton, the main irrigated crop in Arizona, which is irrigated with both surface and groundwater. Water in Arizona is applied to cotton in excess of the crop water deficit, suggesting that a large portion of the applied water runs off the field, percolates to groundwater, or is otherwise remaining in its originating basin (Figure 43). Such water movement from farm to farm within a basin may still be above that needed by the cotton in the basin but is not necessarily in excess for all types of crops in the basin. In this case, if a senior user implements water conservation efforts, it is unclear whether the basin level impact is reduced:

the response of neighboring junior users might be to use more surface or groundwater, the latter at a greater energy expense. Either way, ultimately the water is not conserved. Thus, when using these kinds of water footprinting results to make decisions about land use or crop production, the system boundary must be expanded to include the hydrologic, economic, and political forces governing water use in the region. The consequence of not doing so would be to overestimate the regional impact benefits of conservation measures.

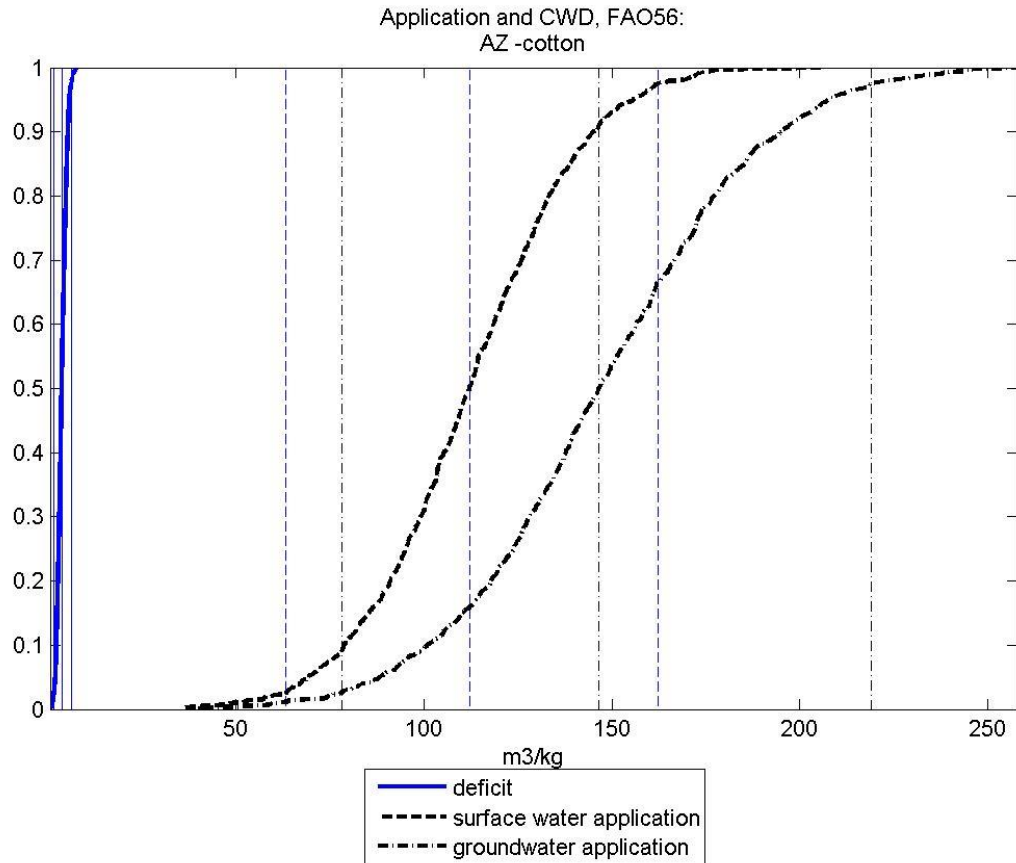


Figure 43: Freshwater application and crop water deficit for cotton grown in Arizona

5.4 Conclusion

There exists large variability in one of the key physical mechanisms for scaling up farm level water consumption impacts—atmospheric recycling. Furthermore, there are uncharacterized levels of uncertainty in the fate of water and its contribution to water stress in regions within the product system boundary. As such, current approaches to

impact – oriented water stress LCIA does not comply with ISO 14044's requirements of: application of characterization models, and analysis of uncertainty for studies used in comparative assertions.

In consideration of the wide range of uncertainty associated with estimating farm level water consumption, and the uncharacterized uncertainty associated with further impact modeling, it is suggested considering using energy as a means of regional impact characterization as opposed to a water stress index. As has been described above, water and energy are closely linked, and the means for estimating energy use for water is straightforward. Energy used for producing water is analogous to a “willingness-to-pay” for a water resource that increases with water scarcity. As a characterization model it is transparent, since it is based on available data and simple physical principles. Although the uncertainty and variability associated with energy use can be large, it is bounded, and can be refined. Further research adapting energy intensity for water production as a characterization model for water scarcity is recommended.

6 Discussion and Conclusions

In practice and with few exceptions, uncertainty analysis in LCA has been comprised of either bounding the results with a series of what-if scenarios, or by varying modeling assumptions such as co-product allocation or offsets.

With freshwater consumption in particular, uncertainty analysis has consisted of varying models used to scale farm level water consumption to impact indicators, and comparing the results (see (Berger and Finkbeiner 2012)). This dissertation has contributed the first estimation of uncertainty for freshwater characterization factors along with farm level consumption estimates—the magnitude of uncertainty and variability associated with the estimate of water consumption characterization factors has been elucidated at small spatial scales. This uncertainty data informs the LCA practitioner in approaches to refinement of the study: for cases where uncertainty of estimates for freshwater consumption are small, and/or there is clear statistical significance between technological alternatives, further iterations of the LCA may not need to include refinement of freshwater consumption data. However, for cases where uncertainty for freshwater consumption is large, and the statistical significance between alternatives is ambiguous, it is recommended that the practitioner either refine the study to reduce the uncertainty, or verify the uncertainty is due to uncertainty in nature as opposed to uncertainty due to gaps in knowledge. The following recommendations are made for reducing uncertainty in estimates of freshwater consumption.

6.1 Recommendations for reducing uncertainty

When considering the larger context of using LCA in support of decision making, we find that the farm scale estimates of uncertainty and variability are but one class of uncertainty associated with making comparative assertions. The following areas of uncertainty and their implications in the context of decision making are outlined in an uncertainty matrix (Figure 44) and are classified by level of knowledge, ranked in order of most knowledge to least (Walker et al. 2005). Statistical uncertainty represents variations described by some type of descriptive statistics, thus there is some knowledge as to the likelihood of the estimate being the actual impact. Scenario uncertainty bounds the variation of the estimates using various ‘what if?’ scenarios or by switching assumptions. Also included is recognized ignorance, areas of uncertainty with an unknown impact on the estimates of the results. The distinction between uncertainty in knowledge and natural variability is also noted, as is the implication of the uncertainty on the estimate.

Figure 44: Uncertainty matrix for estimation of freshwater consumption impact characterization

Category	Characterization factor	Level of uncertainty			Nature of uncertainty		Sensitivity (95% conf.)
		Statistical	Scenario	Ignorance	Knowledge related uncertainty	Variability related uncertainty	Average (as % of estimate)
precipitation	Green and blue water						28
evapotranspiration	Green and blue water						100
crop growing periods	Green and blue water						115
crop yields	Green and blue water						na
irrigation depth	Blue water						18
irrigation efficiency	Blue water						2
atmospheric recycling	Green and blue water						40
control volume - spatial scale	Green and blue water						na
air-surface dynamic feedback	Green and blue water						na

The uncertainty associated with both the precipitation and evapotranspiration estimates, as presented in this dissertation, are statistical uncertainty due to variations in space and time of the associated climate data. However, both categories of parameters are based upon climate re-analyses and estimates, thus they both contain some un-

quantified ignorance associated with the estimate of the data (see (Maurer et al. 2012) for detailed descriptions of data estimates). On average, sensitivity of characterization factors to evapotranspiration is about 100% of the estimate and about 28% of the estimate for precipitation for ± 2 standard deviations of climate data. Refining the spatial scope is recommended to reduce the statistical uncertainty associated with precipitation and evapotranspiration. Refining crop production data to the county or smaller scale, or refining system boundaries to include only those watersheds relevant to specific crop production could reduce natural variability in freshwater consumption estimates.

Variation due to crop growing periods can have a 95% confidence interval larger than the estimate on average for green and blue water consumption. Crop growing periods are spatially resolved to the state level, and the temporal variability is represented as three points describing planting and harvesting dates: 5% complete, most active (assumed to be 50% complete), and 95% complete. Like the climate data, uncertainty associated with crop growing periods can be reduced by refining the spatial scope. Also, uncertainty may be reduced by improving the quality of uncertainty data associated with crop growing periods, perhaps by improved surveys or resampling techniques to develop probability distributions for planting, harvesting, and crop growth rates. For this work, there remains acknowledged ignorance on the impacts and relevance of crop yield and it is recommended that yield variability data be included for future work in developing crop freshwater consumption estimates.

On average, sensitivity to irrigation application data is roughly 20% of the estimate for a 95% confidence interval. Raw data associated with irrigation application is masked to preserve the privacy of survey respondents by performing jack-knife resampling to produce estimates described by a student's t distribution with 15 or 30 degrees of freedom (Kim et al. 2004). The magnitude of the variability due to resampling, as opposed to the variability in actual irrigation application, represents an uncharacterized ignorance. Aside from improving the state level spatial resolution, uncertainty associated with resampling may be reduced or eliminated by finding alternative methods for estimating irrigation application, such as by remote sensing or other geospatial tools. Uncertainty in irrigation efficiency is coarsely modeled here as a triangular distribution of efficiency values based on handbook rules-of-thumb. However, the contribution of irrigation efficiency to freshwater consumption uncertainty is relatively small at about 2% of the estimate on average.

As is described in sections 2.8 *Criticisms and research needs for scaling impact-based approaches* and 4 *Assessing Freshwater Consumption in LCA at the Regional Level*, the estimate of farm level freshwater consumption represents a conservative estimate of the consumption impact due to the role of atmospheric recycling in scaling. Scenario uncertainty includes uncertainty due to temporal variation which can range from 0 – 20% reduction to 0 – 80% reduction in the estimate of freshwater consumption at the farm level, and the impact of length scale which can decrease the estimate of consumption from 10% up to 60% for constant vapor flux and evaporation rates. Substantial effort must be taken to integrate vertical atmospheric water vapor data to solve the water balance equation presented in Equation 37. Thus, it is recommended that the system boundary is first refined to determine which regions could benefit from enhanced estimation of atmospheric recycling uncertainty.

However, aside from the scenario uncertainty described above, there remains uncharacterized ignorance associated with control volume definition, fate of recycled water, and the dynamic coupling between surface land cover and atmospheric water vapor. The appropriate definition of the control volume can have significant implications on the impact of atmospheric recycling. Consider for example the Mississippi Basin in which up to 80% of evaporated water can be recycled within the basin. Water users at the mouth of the Mississippi Delta, the confluence of all of the watersheds in the entire basin, experience the total benefit of atmospheric recycling associated with all upstream activities. However users at the head waters of the Mississippi may not experience any benefit of atmospheric recycling as all recycled water vapor precipitates downstream from those users. Thus the appropriate definition of the control volume is necessary to reduce the ignorance associated with spatial variations in recycled precipitation. Similarly, the fate or the location of recycled water precipitation is necessary to accurately determine the benefit of atmospheric recycling on water consumption impacts. A probabilistic representation of where water goes is necessary to reduce ignorance to a statistical representation of uncertainty in fate of atmospheric water vapor. And finally, there exists a dynamic coupling between the land surface and land cover, and the amount of water that enters the atmosphere. This in turn affects that amount of water that is available locally as precipitation, thus using LCA as a tool for decision making must also consider the changes in impacts associated with changes in land cover. Application of dynamically coupled land surface atmospheric models appropriate to the region of interest (such as that described by (Subin et al. 2011) for example) could be applied to ascertain the significance of land cover change on freshwater consumption impacts. However, there also exists some amount of ignorance associated with the

veracity and relevance of models used in forecasting, and refinement of approaches using increasingly sophisticated models may introduce new, uncharacterized uncertainties.

6.2.1 Conclusions, Chapter 2 Research Goals, Motivation, and Broader Impacts

Current approaches employed to characterize impacts to freshwater scarcity, beyond basic inventories, do not comply with ISO 14044. Volumetric approaches, such as those of Hoekstra et al. employ an arbitrary scaling factor to green, blue, and grey water consumption to produce total water footprints (A. Hoekstra et al. 2011). Current impact-based approaches, such as (Pfister, Koehler, and Hellweg 2009) neglect regional scale climate dynamics and feedback when scaling up farm level mid-point indicators. In addition, there is as of yet, no characterization of climate variability or model uncertainty in the production of water consumption impact models. Thus, at this time, comparative assertions between technologies, based on freshwater impacts, cannot be made with any degree of reliability.

6.2.2 Conclusions, Chapter 3 Assessing Water Consumption on-site

Uncertainty and variability for the estimation of farm level green and blue water consumption can be substantial. In particular, the ranges of results due to climate and spatial variability are dramatic, reinforcing the need to include uncertainty and variability in LCAs making comparisons between technologies. Furthermore, although typically uncertainty analysis in LCIA will be composed of only varying modeling assumptions, here we find the level of uncertainty associated with model choice is small compared to the level of climactic variability. Although there is an increase in work load, the data required to include variability in farm level impact characterization is available.

6.2.3 Conclusions, Chapter 4 Assessing Freshwater Consumption in LCA at the Regional Level

Current approaches to scaling farm level mid – point consumption to regional consumption neglect key environmental mechanisms. The inclusion of atmospheric water recycling as a characterization model introduces another level of complexity and uncertainty, for which the science and the data are not at a level applicable for impact assessment.

6.2.4 Conclusions, Chapter 5 Beyond Water Stress: investigating the water – energy nexus

Water and energy use are closely connected and can be modeled using straightforward physical principles. It is proposed that using energy for water procurement, analogous to a willingness to pay for a water resource, could be a more defensible approach to impact characterization, and is recommended for future work.

6.3 Conclusions: Overall

The quantification of uncertainty and variability is a critical element in assessing freshwater consumption impacts in particular, and LCA in general. For LCAs making comparative assertions, sensitivity and uncertainty analysis is necessary, not just for ISO compliance, but also to establish the significance of the differences between alternatives, and to improve the reliability and veracity of results. Furthermore, performing uncertainty analysis can help reveal the appropriateness of applying particular characterization models and methods to environmental inventories. LCIA methods with unbounded or unquantified uncertainty should be avoided, despite what would appear to be a logical map of impact pathways, in favor of approaches that are repeatable and technically defensible.

Presently available LCIA methodologies are static in nature; they are backwards looking in time, and represent average, status quo conditions over large spatial areas, and for generic conditions. Improved confidence in LCIA methodologies and LCA results requires defining system boundaries specifically as defined in the goal and scope phase of each LCA. Thus, relevant LCIA methods require characterization models that can be applied in concert with LCA studies, such as integrating fate and transport models such as Daycent³¹ for soil carbon and nitrogen, PestLCI for pesticides (Birkved and Hauschild 2006), and hydrological models such as VIC (Liang et al. 1994). In developing LCA, uncertainty has been neglected in an effort to focus on fundamental concepts and methods. However, as the science has matured and availability of data has improved, the time of LCA for making high level policy decisions has arrived, and with it the need for robust and reliable data, complete with representations of uncertainty.

³¹ See: <http://www.nrel.colostate.edu/projects/daycent/>

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