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## ▶ To cite this version:

Wenjie Liao, Hayo van Der Werf, Jordy Salmon-Monviola. Modelling of nitrogen releases in life cycle assessment of crop production. the 9th International Conference on Life Cycle Assessment in the Agri-Food Sector, Oct 2014, San Francisco, United States. pp.718-724. hal-01209241

## HAL Id: hal-01209241 https://hal.science/hal-01209241v1

Submitted on 2 Jun2020

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### Modelling of nitrogen releases in life cycle assessment of crop production

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#### ABSTRACT

The modelling of reactive nitrogen (Nr) releases poses a big challenge to the life cycle assessment (LCA) of crop production. This study aims at providing an overview of potential aspects that need to be taken into account for improved modelling of Nr releases in the LCA of crop production. The definition of a crop product system and considerations of the crop, the soil, and the spatial scale were revisited. The major pathways of releases of nitrate, nitrous oxide, and ammonia were distinguished. Empirical emission-factor-based methods and process-based models for the development of unit process dataset of on-site crop production were summarised and compared. The importance of modelling fates of Nr releases was discussed. At the end, several conclusions were drawn.

Keywords: nitrate, nitrous oxide, ammonia, release, crop production

#### 1. Introduction

Crops are plants that can be grown and harvested extensively for profit or subsistence (Encyclopædia Britannica 2014). Crop production, whist contributing to ensuring ample food and feed supply and enabling adequate farmer income, has induced numerous detrimental impacts on the quality of air, water, and soil, terrestrial ecosystems and biodiversity, greenhouse gas balance, etc. (Tilman 1999; National Research Council 2010). Crop production is the single largest cause of human alteration of the global nitrogen cycle (Liu et al. 2010). Life cycle assessment (LCA) has been identified as a valuable tool for the evaluation of potential environmental impacts of farming systems (van der Werf and Petit 2002) and applied increasingly to crop production as well as animal production (Brentrup et al. 2001; Haas et al. 2001; Bessou et al. 2013; Perrin et al. 2014).

However, originally developed for industrial production, the application of LCA to crop production faces challenges, which are determined by the features of crop production that are more complicated than industrial production. A main complicating feature is that crop production uses the soil. The dynamics of crop nutrients such as nitrogen, phosphorus, and potassium as controlled by biophysical soil processes need careful consideration (Harris and Narayanaswamy 2009). The development of models to estimate on-site pollutant emissions of crop production has been identified as a topic that leads the methodological development in LCA (van der Werf et al. 2014).

Amongst crop nutrients, nitrogen is of crucial importance, as it is a major determinant of crop growth and yield (Goulding et al. 2008). The large increases in reactive nitrogen substances (Nr) as fertilisers used in crop production, observed after the Second World War in many parts of the world, have triggered a cascade process generating Nr releases to air, soil, and water at each stage of the cascade (Galloway et al. 2003). Nr have been systematically catalogued in life cycle inventory (LCI) results and assessed against several important potential environmental impacts in life cycle impact assessment (LCIA).

The aim of this study is to provide an overview of potential aspects that need to be considered for improved modelling of Nr releases in the LCA of crop production.

#### 2. Goal and scope definition

#### 2.1. The crop product system

In LCA studies the boundary should be delineated clearly between the product system and the ecosphere. In the LCA of crop production, a crop product system encompasses both the upstream processes, i.e., the extraction of natural resources and the supply chain of various intermediate products such as fertilisers, pesticides, machinery, infrastructure, energy, etc., and the on-site crop production. The crop delivered at the farm gate is used for several possible functions such as food, livestock fodder, biofuel stock, clothing, medicine, etc. (A

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detailed classification of crops and crop functions can be found in the FAO World Programme for the Census of Agriculture (2010)).

The analysis of on-site crop production involves modelling consideration in three dimensions, vertically about the crop and the soil and horizontally about the spatial scale. The harvested portion of the crop and the remaining non-harvested portion are regarded as part of the product system and part of the ecosphere, respectively. Soil can either be included in the ecosphere based on the hypothesis that damage to the soil should be regarded as an environmental impact so as to distinguish systems differing in their impacts on soil quality, as suggested by Wegener Sleeswijk et al. (1996), or be regarded as an integral part of the product system, as proposed by Audsley et al. (1997). This study follows Audsley et al. (1997) to take into account the crop and the soil with a depth right down to the water table, which is location specific and changes along with seasons, in delineating the crop product system. On-site crop production can be modelled and analysed on a range of spatial scales, from the field through the farm to the farming region or even broader scales (e.g., a nation). The different spatial scales may include different compartments of the ecosphere and thus imply different fates of Nr releases in the assessment.

#### 2.2. Major Nr under consideration

A non-exhaustive list of various forms of Nr under consideration in LCA studies is provided in Table 1.1. The three most important Nr releases in the LCA of crop production are nitrate  $(NO_3^-)$ , nitrous oxide  $(N_2O, a.k.a. dinitrogen oxide)$ , and ammonia  $(NH_3)$ , which contribute to the impact categories of terrestrial and aquatic eutrophication, climate change, and acidification.

1.0	verview of federive	The world reactive introgen substances and then contributed environmental impacts in Derr			
	Nr Substance	formula	Impact category		
	Nitrate	NO3 <sup>-</sup>	Eutrophication		
	Nitrite	NO <sub>2</sub> -	Eutrophication		
	Ammonia	NH <sub>3</sub>	Acidification and eutrophication		
	ammonium	$NH_{4}^+$	Acidification and eutrophication		
	Nitrous oxide	$N_2O$	Climate change and ozone depletion		
	Nitrogen oxides	NOx	Acidification, eutrophication and photochemical ozone formation		

Table 1. Overview of reactive nitrogen substances and their contributed environmental impacts in LCA

#### 2.2. Pathways of Nr releases

Based on the aforementioned definition of a crop product system, two types of Nr releases can be distinguished: upstream Nr releases and on-site Nr releases, which are elementary flows from the crop product system to the ecosphere. Upstream releases are associated typically with inputs to the on-site production, for instance, the release of NOx due to fuel use. Their data are usually obtained from existing databases such as ecoinvent (Swiss Centre of Life Cycle Inventories 2010). Whilst increased Nr mineralisation/nitrification can be a significant source, on-site releases are mainly due to the applied nitrogen fertilisers, which are transformed and transferred in the soil and taken up by crops that are modelled as part of the product system. Crop residues can be a major contributor to the release of N<sub>2</sub>O (Baggs et al. 2000). Most on-site Nr releases are attributed to a range of transformations including ammonia volatilisation, nitrification and denitrification, and to the transfer in terms of nitrate runoff and leaching and organic Nr runoff, as shown in Figure 1 (Parnaudeau et al. 2012) (Note that processes of exportation and fixation in Figure 1 are actually outside of the crop product system).

Outside of the crop product system, upstream and on-site Nr releases experience various transformations and affect the environmental quality and human health. These transformations correspond to the cause-effect chain between releases and environmental impacts and are the basis for modelling nitrogen-related impacts in LCIA. Table 2 summarises the major pathways that are within and outside of the crop product system.

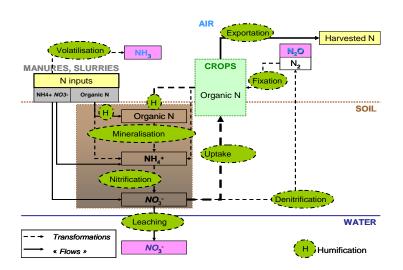


Figure 1. Nr releases from the on-site crop production (Parnaudeau et al. 2012)

	Table 2. Overview of	pathways of Nr releases	related to crop pr	oduction
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Nr	Within crop produc	t system	Outside crop product system	
	Upstream release On-site release		Transformation	
NO <sub>3</sub> -	Discharge	Leaching and runoff	Denitrification, ammonification	
N <sub>2</sub> O	Emission	Denitrification of NO <sub>3</sub> <sup>-</sup> in soil, crop residues	Denitrification, nitrification	
NH <sub>3</sub>	Emission	Volatilisation	Nitrification	

#### 3. LCI related to Nr releases

Nr release rates can vary greatly depending on farmer practices, weather conditions, soil characteristics, landscape characteristics, hydrological processes, etc. (IFA/FAO 2001). On-site measurements of the Nr releases are costly and time-consuming, and in any case display great variations, because they only reflect a snapshot of the specific conditions of the on-site crop production at the time of measurement (Brentrup et al. 2000). In practice, the unit process dataset of on-site crop production is seldom built based on on-site measurements but rather created by linking raw data from various sources with pertinent mathematical relationships. Two types of mathematical relationships are distinguished, i.e., empirical emission-factor-based methods and process-based models.

#### 3.1. Empirical emission-factor-based methods

An emission factor (EF) is defined as the average emission rate of a given (gaseous) pollutant for a given source, relative to units of activity. Emission factors are traditionally used to quantify air, water and soil pollutants at relatively high aggregation levels (e.g., the national scale), rather than at the individual source of emissions. In most cases, these factors are simply averages of all available data of acceptable quality. For instance, a default EF of 0.01 (range: 0.3-3%) was suggested by the Intergovernmental Panel for Climate Change (IPCC, 2006) to calculate the N<sub>2</sub>O emission due to fertiliser application to managed soil at the national scale.

Bessou et al. (2013) and Perrin et al. (2014) reviewed 155 publications on perennial crop production and 17 publications on vegetable crop production, respectively. Three common references were identified as the general guidelines in estimating "field emissions" (i.e., on-site Nr releases), viz. Audsley et al. (1997), Nemecek and Kägi (2007), and Brentrup et al. (2000), as summarised in Table 3. In addition, the 4th report of the Intergovernmental Panel for Climate Change (IPCC, 2006) was also identified as an important guideline for perennial crops by Bessou et al. (2013).

, DC	Dessou et al. (2013) and Ferrin et al. (2014))				
	Nr Audsley et al. (1997)		Brentrup et al. (2000)	Nemecek and Kägi (2007)	
	NO <sub>3</sub> -	n.a. <sup>a</sup>	N-NO <sub>3</sub> -,soil	n.a. <sup>a</sup>	
	$N_2O$	EF% of N <sub>fertiliser</sub>	EF=1.25% Nfertiliser- NH3loss	EF=1.25% Nsoil	
	NH3,fertiliser	EF% of N <sub>fertiliser</sub>	EF% of N <sub>fertiliser</sub>	EF% of N <sub>fertiliser</sub>	
	NH <sub>3,manure</sub>	EF=50% of N-NH4,manure	N-NH <sub>4,manure</sub>	N-NH <sub>4,manure</sub>	

Table 3. Empirical emission-factor-based methods for estimating on-site Nr releases of crop product systems (following Bessou et al. (2013) and Perrin et al. (2014))

<sup>a</sup>n.a.: not available in English.

#### 3.2. Process-based models

Process-based models try to represent physical/biological/hydrological processes observed in the reality (Korzukhin et al. 1996). They are spatialised (semi-distributed or distributed) models, which can take into account different scales of representation of crop production (field, farm, farming region, etc.) and the interactions between the subsystems of the crop product system. Typically, for the estimation of releases from crop production such models contain representations of surface runoff, subsurface flow, evapotranspiration, and channel flow. Process-based models are increasingly recognised as alternatives to empirical emission-factor-based methods. We selected several process-based models through a search for peer reviewed English publications in the ISI Web of Knowledge (accessed on 9 April 2014), which is summarised in Table 4.

Table 4. Selected process-based models for estimating Nr releases from crop production

Process-based model a	Reference	Simulated Nr	Scale
CERES-EGC	Gabrielle et al. (2006),	N <sub>2</sub> O	Farming region
	Bessou et al. (2013)		00
DNDC	Li (2000)	NO3 <sup>-</sup> , N2O, NH3	Farming region, nation
	Deng et al. (2011)		
DayCent	Parton et al. (1998),	N <sub>2</sub> O, NO <sub>x</sub>	Farming region
	Del Grosso et al. 2005)		
DNMT	Liu et al. (2005)	NO <sub>3</sub> -	Farming region
SWAT	Arnold et al. (1998),	NO <sub>3</sub> -	Farming region
	Gramig et al. (2013)		
FASSET	Jacobsen et al. (1998),	NO <sub>3</sub> <sup>-</sup> and NH <sub>3</sub>	Field, farm
	Chatskikh et al. (2005)		
HERMES	Kersebaum (2007)	NO <sub>3</sub> <sup>-</sup> and NH <sub>3</sub>	Field
TNT2	(Beaujouan et al. 2002)	NO <sub>3</sub> -, NH <sub>3</sub>	Farming region
INCA	(Wade et al. 1999)	$NO_3^-$ , $NH_4^+$	Farming region

<sup>a</sup> CERES-EGC: Crop Environmental REsources Synthesis; DNDC: DeNitrification-DeComposition; DayCent: Daily Century; DNMT: Diffuse Nitrate Modelling Tool; SWAT: Soil and Water Assessment Tool; FASSET: An Integrated Economic and Environmental Farm Simulation Model; TNT2: Topography-based Nitrogen Transfer and Transformation; INCA: Integrated Nitrogen in Catchments model

As two types of mathematical relationships to create unit process datasets from raw data, empirical emissionfactor-based methods and process-based models differs for several characteristics, as indicated in Table 5. Process-based model can simulate the Nr dynamics related to the crop product system by parameterising various influencing mechanisms. Data representativeness and model uncertainty depend on the data availability, which will often determine which approach is used. Whenever sufficient data are available, process-based models are recommended. However, special attention should be paid to ensure the consistent spatial scale of stand-alone LCA studies of crop production and those coupled with process-based models.

Table 5. Comparison between empirical emission-factor-based methods and process-based models in LCA of crop production.

Characteristic	Empirical emission-factor based methods	process-based models	
Mathematical relationship	Stochastic	Deterministic	
Data requirements	lower	Higher	
Data representativeness	lower	Higher	
Primary error source	Extrapolation	Unknown parameters	
Model uncertainty	Lower	Higher	

#### 4. LCIA related to Nr releases

The fate of an on-site Nr release consists of its transfer, transformation, and accumulation or dilution in a compartment of the ecosphere (Basset-Mens et al. 2006). The fate of a specific release plays an important role in the cause-effect chain linking its release to its potential environmental impacts and needs to be carefully modelled. Considering the aforementioned definition of the crop product system, such a compartment can be the atmosphere, the hydrosphere, or part of the pedosphere that is not included in the crop product system. The formation of N<sub>2</sub>O outside of the crop product system (cf. Table 2) indicates that the fate factors of leached NO<sub>3</sub><sup>-</sup> and volatilised NH<sub>3</sub> from the on-site crop production are both intrinsically inferior to 1 in the hydrosphere and the atmosphere, respectively. Fates of an Nr releases are usually ignored by assuming them equal to 1 excepted in rare studies such as Basset-Mens et al. (2006). Basset-Mens et al. (2006) looked into the fate factors of NO<sub>3</sub><sup>-</sup> releases in three different catchments in west France, based on the fate factor for NO<sub>3</sub><sup>-</sup> which was defined as the ratio of the NO<sub>3</sub><sup>-</sup> quantity at the outlet of a catchment over the NO<sub>3</sub><sup>-</sup> discharged from the catchment's soils. It can be a valuable reference for future studies on simulating the fate, for instance, of NH<sub>3</sub>.

#### **5.** Conclusion

The following aspects need to be taken into account for improved modelling of Nr releases in the LCA of crop production:

- The crop product system consists of upstream processes and the on-site crop production. The on-site crop production includes the harvested portion of the crop and the soil with a changing depth down to the water table
- Nitrate, nitrous oxide, and ammonia are three important reactive nitrogen substances under consideration. They should be distinguished within the crop product system and between the crop product system and the ecosphere.
- Empirical emission-factor-based methods and process-based models are typical approaches for the development of unit process dataset for on-site crop production. Stand-alone LCA studies of crop production and those coupled with process-based models should be based on the consistent spatial scale.
- Fates of reactive nitrogen releases in the ecosphere should be explicitly modelled in the life cycle impact assessment phase of the LCA of crop production.

#### Acknowledgements

W. L. has received the support of the European Union, in the framework of the Marie-Curie FP7 COFUND People Programme, through the award of an AgreenSkills' fellowship (under grant agreement n° 267196).

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# Proceedings of the 9th International Conference on Life Cycle Assessment in the Agri-Food Sector



8-10 October 2014 - San Francisco

Rita Schenck and Douglas Huizenga, Editors American Center for Life Cycle Assessment The full proceedings document can be found here: http://lcacenter.org/lcafood2014/proceedings/LCA\_Food\_2014\_Proceedings.pdf

It should be cited as:

Schenck, R., Huizenga, D. (Eds.), 2014. Proceedings of the 9th International Conference on Life Cycle Assessment in the Agri-Food Sector (LCA Food 2014), 8-10 October 2014, San Francisco, USA. ACLCA, Vashon, WA, USA.

Questions and comments can be addressed to: staff@lcacenter.org

ISBN: 978-0-9882145-7-6