TECHNICAL SUSTAINABILITY OF BIOLOGICAL PRODUCTION SYSTEMS

A MODEL BASED LIFE CYCLE ASSESSMENT OF FERTILIZER MANAGEMENT

Reindert HEUTS

Supervisors:
Prof. Dr. E. Schrevens
Prof. Dr. J. Diels

Members of the Examination Committee:
Prof. Dr. J. Van Orshoven
Prof. Dr. H. Ramon
Prof. Dr. R. Merckx
Prof. Dr. B. Muys
Prof. Dr. C. Bojacá

Dissertation presented in partial fulfilment of the requirements for the degree of PhD in Bioscience Engineering

June 2018

Doctoraatsproefschrift nr. 1520 aan de faculteit Bio-ingenieurswetenschappen van de KU Leuven

Uitgegeven in eigen beheer, REINDERT HEUTS, MECHELEN

Acknowledgements

This doctoral work was realized along the IWT-funded project *ECOFert*: ‘Online monitoring and model-based support system for just-on-time N fertilization in open field horticulture’.

Thank you very much to each and all of you who joined me on the road towards my PhD.

First of all, thank you, Eddie, my promotor, for your guidance. The no-nonsense, the openness, the patience, the confidence... a good mix and nice atmosphere at the office.

Also thank you, Jan, my co-promotor, for the dedication.

Much appreciation goes to the examination committee for their valuable and constructive comments and suggestions, making this a better work.

Thank you, Jelle and Joachim, my ex-colleagues, for the laughs, doubts and drinks and for the smell of drying cauliflower and leek, shared with the whole campus.

Thanks, my Peruvian gang, Ximena, Diego, Diana and Cindybell, allowing me to be ‘el jefe’ occasionally. Also thanks to my Colombian friends, Carlos and Rodrigo, for the amazing time abroad.

Thank you, friends and family, mam, dad and sis, for the unconditional support and diversion. It kept me going.

Kim, my love, thank you, always, I owe you big time.

Thank you, Jasmijn en Mona, my ladies-in-crime, for your stimulating smiles.

Summary

Accordingly with world's movement towards sustainable development, agriculture faces mounting pressure to reduce its environmental impact. The present organisation of our food production leads to significant alterations of the global nitrogen cycle causing increased nitrogen emissions into the ecosystem. Aiming at sustainable systems requires to account for long-term implications of practices and the broad interactions and dynamics of agricultural processes. A key goal hereby is to pursue technical sustainability through understanding agriculture from a biophysical perspective in terms of water and nutrient dynamics, and interactions among plant and soil under changing climate conditions and different management strategies. The present work provides an integrated dynamic and process based crop-soil model which is coupled to a life cycle assessment (LCA) to evaluate the technical sustainability of a biological production system. The model simulates crop growth and development as well as soil water and nitrogen dynamics under varying climate conditions and different nitrogen fertilizer application rates. With this dynamic approach to predict the related field nitrogen emissions, a more reliable and realistic assessment of the environmental impact can be obtained to enhance the by default static LCA output. This allowed the assessment of implications of future management scenarios considering potential impact reduction strategies. More specifically, the open field production of a cauliflower leek rotation in Flanders, Belgium was chosen as case study throughout the whole research. It is a commonly applied rotation cycle susceptible for excessive use of inorganic fertilizers.

A life cycle assessment, a widely recognized method within the sustainability assessment, quantifies the environmental impact of a system in terms of impact categories like global warming, eutrophication, toxicity, etc. An LCA provides a comprehensive and objective method of analysis that identifies the environmentally most dominant stage(s) in a product life cycle and allows the comparison of alternative production (sub)systems regarding their environmental burden. A preliminary LCA with commonly used empirical models to estimate the field emissions, showed that increased fertilizer application does not result in a sufficient increase in yield to justify additional emissions and to be environmentally favourable. Application of a lower N dose would benefit the environment, but entails a lower commercial yield. It would be a matter of finding the trade-off between yield and potential environmental costs, as the land occupation favours the higher N doses. Although, the latter is not necessarily true in terms of only the edible part of the crop compared to the commercial yield of the whole crop as functional unit. In any case, besides potential renewable energy sources, efforts should be made to reduce emissions of nitrogen pollutants as they are a major source for climate change, acidification and eutrophication. The empirical approach for their calculation however, is very limited to account for

the potential effect of mitigation strategies due to the aggregated estimation level and the lack of predicting their implications on crop growth and soil conditions. As natural variability due to varying biophysical conditions is inherent in agricultural production, future climate and soil conditions could alter the whole nitrogen flow through the crop-soil-air environment and shift the most favourable fertilizer management. Although LCA is praised for its holistic approach, it has an inherent static and linear nature and heavily depends on the quality of input data.

Therefore, driven by meteorological data, soil properties and agricultural management, a crop-soil- climate interaction model was developed which simulates at field scale on a daily basis the soil temperature, crop growth and development, water flow and soil carbon and nitrogen dynamics including emissions of environmental pollutants to the air and ground water. If the soil supply of water and/or nitrogen does not meet the demand of the crop, a deficiency factor is implemented to limit crop growth and actual water and nitrogen uptake. According to the visual match and associated statistical performance indicators, model predictions were fair to very good as well for the calibration as for the validation with three years of observations and different N dose rates. Given the large variability and strict performance rating thresholds, biomass growth, its nitrogen content, the water content and temperature in the different soil layers predicted the observations very well. The soil nitrogen content simulation however suffered from the discrete limited sampling numbers, the lack of detailed knowledge and the complex interaction of different pathways that affect the content simultaneously. Along with the calibration, a local sensitivity analysis of the model responses to changes in model parameters was performed based on the ratio of their coefficients of variation. Certain soil processes, especially runoff, water percolation and nitrogen leaching and the emission of nitrous oxides were found to be sensitive to a 10% change of mainly the runoff curve number for average moisture content and the water content at field capacity of the top layer.

Next, the LCA results were compared with nitrogen field emissions estimated by either the default empirical approach or by the developed dynamic model. Overall, the model based LCA showed a consistently lower impact than the default LCA results of the same crop rotation cycle and fertilizer management. The only exception was the eutrophication potential under the higher N dose application rates for all three years. Differences between the impacts according to both approaches tend to increase with increasing N dose rate besides the impact itself. Changes of impact over the different years were reflected similarly by both outcomes. However, as the empirical approach might look straightforward regarding alternative solutions, they are limited and potentially ineffective. If the LCA needs to support future management decisions, an appropriate choice of approach for estimating field nitrogen emissions is required as it might shift the environmental favourable option to alternative and substantiated solutions, especially considering the timing of reduction strategy implementation. A daily time step and accounting for multiple processes and disturbing factors allows the model based simulation to provide more accurate and efficient adaptations towards sustainable systems. Furthermore, the implications of management adjustments or extreme climate changes on crop yield and nitrogen dynamics cannot be addressed by the default LCA method as the empirical approach depends on standard crop N uptake curves and does not account for precipitation and soil moisture effects for instance. In a dynamic system like the water and nitrogen flow in a crop-soil environment, impact assessment should address 'when' even more than 'which' potential reduction strategies should be implemented.

Finally, the model based LCA was implemented for a scenario analysis that included potential reduction strategies regarding fractionated fertilizer application and plastic mulching during winter fallow periods. Whereas a fertilizer application distributed in time to meet the crop demand might reduce N stress and increase yield, the winter soil cover could prevent drain and subsequent nitrogen leaching. Although this was to a certain extent reflected in the outcome of the model simulations, the mitigated environmental impact was cancelled by the burden from additional fertilizer equipment and energy use and/or especially from the plastic cover production and disposal. Only the eutrophication potential would be reduced if the strategy would be implemented. It shows that future decisions require a holistic perspective that combines dynamic model predictions and aggregated LCA results, which still would imply a trade-off between different impacts, but would prevent a problem shift. Such scenario analysis is considered less reliable and could be more misleading with the empirical approach as applied in default LCA studies regarding dynamic agricultural systems.

The current implementation of the model based life cycle assessment showed the strength and importance of a system analysis to (i) provide improved process based insight in the agricultural production system with more reliable predictions, (ii) to understand, quantify and optimize the technical sustainability of a product and (iii) to address more complex issues on sustainable production and future decisions.

Samenvatting

De globale evolutie naar duurzame ontwikkeling induceert ook een stijgende druk op de landbouw om zijn milieu-impact te verlagen. De huidige organisatie van onze voedselproductie leidt tot significante wijzigingen in de stikstofcyclus met toenemende stikstofemissies in ons ecosysteem als gevolg. Duurzame systemen vereisen rekening te houden met lange-termijn implicaties van landbouwpraktijken en de brede interacties en wisselwerking van biochemische landbouwprocessen. Het hoofddoel hierbij is de technische duurzaamheid na te streven door het landbouwsysteem te bekijken en begrijpen vanuit een biofysisch perspectief in termen van water en nutriënten dynamica en de interactie tussen plant en bodem onder wijzigende weersomstandigheden en verschillende beheersstrategieën. In deze studie werd een geïntegreerd dynamisch en procesgebaseerd gewas-bodem-klimaat-interactie model ontwikkeld dat gekoppeld werd aan een levenscyclusanalyse (LCA) om de technische duurzaamheid van een biologisch productiesysteem te evalueren. Het model simuleert de plantgroei en ontwikkeling en ook de water- en stikstofdynamica in de bodem onder wijzigende weersomstandigheden en verschillende stikstof bemestingstoepassingen. Met deze dynamische benadering om de stikstofemissies te voorspellen, kan een meer betrouwbare, realistische en procesgebaseerde beoordeling gemaakt worden ter verbetering van de standaard statische LCA output. Dit laat toe om implicaties van toekomstige beleidsscenario's te evalueren met betrekking tot potentiële impactreductiestrategieën. Als casestudie werd het volledige onderzoek toegepast op een vollegrondsgroentenrotatie van bloemkool-prei in Vlaanderen, België. Het is een veelvoorkomende rotatiecyclus die gekenmerkt wordt door een overdadig gebruik van kunstmeststof.

Een levenscyclusanalyse, een alom erkende methode binnen de duurzaamheidsanalyse, kwantificeert de milieu-impact van een systeem in termen van impactcategorieën zoals klimaatsverandering, eutrofiëring, toxiciteit, etc. Een LCA omvat een uitgebreide en objectieve methode die de meest milieubelastende fase in de levenscyclus van een product identificeert en toelaat om alternatieve productie (sub)systemen te vergelijken naar hun milieu-impact toe. Een standaard LCA met algemeen toegepaste empirische modellen om stikstofemissies te schatten, toonde aan dat toenemende meststofdosissen onvoldoende resulteerde in een meeropbrengst om de bijkomende emissies te rechtvaardigen en milieugunstig te zijn. Toepassing van een lagere stikstofdosis zou het milieu ten goede komen, maar houdt wel een lagere commerciële opbrengst in. Dit impliceert een balans te vinden tussen opbrengst en potentiële milieukosten, gezien het landgebruik gunstiger is onder de hogere stikstofdosis. Dit geldt echter niet noodzakelijk in functie van enkel het eetbaar gedeelte van de gewassen in vergelijking met de commerciële oogst als functionele eenheid voor de LCA. In elk geval, naast potentiële hernieuwbare energiebronnen, dient er inspanning geleverd te worden om emissies van stikstof te reduceren aangezien zij een belangrijke impact hebben naar klimaatsverandering, verzuring en eutrofiëring toe. De empirische benadering is niet de optimale methode om het potentiële effect van mitigatiestrategieën na te gaan ten gevolge van het geaggregeerde schattingsniveau en het gebrek aan voorspellingskracht inzake implicaties voor gewasgroei en bodemcondities. Natuurlijke variabiliteit tengevolge van variërende biofysische condities, is inherent aan landbouwproductie waarbij toekomstige weers- en bodemomstandigheden de hele stikstofcyclus doorheen het gewas-bodem-atmosfeer-systeem kunnen wijzigen en het meest gunstige bemestingsbeheer doen verschuiven. Hoewel de LCA geloofd wordt om zijn holistische aanpak, is het steeds statisch en lineair van aard en enorm afhankelijk van de kwaliteit van input gegevens.

Daarom werd, voorzien van meteorologische data, bodemeigenschappen en landbouwbeheer, een gewas-bodemmodel ontwikkeld dat op veldschaal en dagelijkse basis de bodemtemperatuur simuleert, de gewasgroei en ontwikkeling, het watertransport en de organische koolstof- en stikstofdynamica met inbegrip van verontreinigende emissies naar de lucht en het grondwater. Indien de bodemvoorraad van water en/of stikstof niet voldoet aan de vraag van de plant zal een deficiëntiefactor de gewasgroei en effectieve water- en stikstofopname beperken. Volgens de visuele evaluatie met bijhorende statistische performantie-indicatoren stemden de modelvoorspellingen voldoende tot zeer goed overeen met de observaties tijdens de kalibratie en validatie voor het driejarige experiment onder verschillende stikstofdosissen. Gezien de grote variabiliteit en strikte performantiedrempelwaarden werden de simulaties van biomassa aangroei, de bijhorende stikstofopname, het bodemwatergehalte en de bodemtemperatuur zeer goed voorspeld. De resultaten voor de bodemstikstofgehaltes echter leden onder de beperkte staalnames, het gebrek aan gedetailleerde kennis en de complexe interactie van verschillende processen die simultaan de stikstofvoorraad beïnvloeden. In de kalibratiestap werd bovendien een lokale gevoeligheidsanalyse uitgevoerd van de model output op een verandering in model parameters gebaseerd op de verhouding van hun variatiecoëfficiënten. Bepaalde bodemprocessen, zoals oppervlaktewaterafvloeiing, water percolatie en stikstofuitloging en de emissie van distikstofoxide, werden sensitief bevonden voor een 10% wijziging in hoofdzakelijk de afvloeiingcoëfficiënt (‘runoff curve number’) en het watergehalte op veldcapaciteit in de toplaag.

Vervolgens werden de LCA resultaten vergeleken met betrekking tot de stikstofemissies enerzijds geschat met de empirische benadering en anderzijds met het ontwikkelde model. Algeheel vertoonde de modelgebaseerde LCA consequent een lagere impact dan de standaard LCA resultaten voor dezelfde gewasrotatie en bemestingsbeheer. De enige uitzondering gold voor de eutrofiëring onder de hoge stikstofdosissen voor de opeenvolgende jaren. Verschillen tussen de impacts volgens beide benaderingen vertonen een toename met stijgende stikstofdosis buiten de impact op zich. Beide benaderingen voorspellen een gelijkaardige impact over de jaren heen. De empirische benadering mag dan wel rechtuit zijn met betrekking tot alternatieve oplossingen, ze zijn dan eerder beperkt en potentieel ondoeltreffend. Als de LCA toekomstige beheersbeslissingen moet ondersteunen, is een geschikte keuze voor de schattingsmethode van stikstofemissies vereist. De meest milieugunstige optie kan immers verschoven worden naar een betere en onderbouwde oplossing, in het bijzonder met betrekking tot de timing van reductiestrategien. Een dagelijkse tijdstap en het opnemen van verschillende processen en storingsfactoren stelt het model in staat meer accurate en efficiëntere aanpassingen aan te geven met het oog op een duurzaam systeem. Bovendien kan de standaard empirische LCA op basis van gestandaardiseerde opname curves en het gebrek aan neerslag- en vochtgehaltefactoren, geen rekening houden met implicaties van beheersaanpassingen of extreme weersveranderingen op de gewasgroei en stikstofdynamica. In een dynamisch systeem van water- en stikstofstromen in een gewas-bodemomgeving, zou de impactanalyse bovenop de potentiële reductiestrategieën zelf ook diens timing moeten bepalen.

Finaal werd de model gebaseerde LCA toegepast voor een scenarioanalyse met betrekking tot gefractioneerde bemesting en het aanbrengen van een soort kunststofdoek tijdens de winter braakperiode als potentiële reductiestrategie. Een gespreide bemesting beter afgestemd op de vraag van het gewas, zou de stikstofstress kunnen reduceren en de oogst verhogen, terwijl de kunststofdoek overtallige drainage in de winter zou voorkomen en bijgevolg de stikstofuitloging verminderen. Hoewel dit tot op zekere hoogte werd voorspeld door de model simulatie, werd de gemitigeerde milieu-impact teniet gedaan door de bijkomende schade van bemestingsmateriaal en –energieverbruik en/of voornamelijk door de schade wegens kunststofproductie en diens afvalverwerking. Enkel de eutrofiëring zou gereduceerd worden bij het implementeren van de reductiestrategie. Het toont aan dat toekomstig beleid een holistisch perspectief vereist dat de dynamische modelvoorspellingen combineert met de geaggregeerde LCA resultaten, hetgeen nog steeds een afweging inhoudt van de verschillende impactcategorieën, maar wel een probleemverschuiving voorkomt. Dergelijke scenarioanalyses op basis van de standaard empirische LCA worden beschouwd als minder betrouwbaar en zelfs misleidend met betrekking tot dynamische landbouwsystemen.

De huidige implementatie van de modelgebaseerde LCA heeft de sterkte en het belang van een systeemanalytische aanpak aangetoond om (i) een verbeterd, procesgebaseerd inzicht in het landbouwproductiesysteem bij te brengen met meer betrouwbare voorspellingen, (ii) om de technische duurzaamheid van een product te vatten, te kwantificeren en te optimaliseren en (iii) om meer complexe kwesties inzake duurzame productie en gerelateerde toekomstige beslissingen te onderzoeken.

List of Figures

α	Transfer coefficient of C between SOM pools [-]
γ	Psychometric constant [kPa / °C]
§	Scaling factor for soil water regarding damping depth [-]
Δ	Rate of change of the saturated vapour pressure with air temperature [kPa / °C]
φ_l	Soil layer porosity [-]
θ	Soil water content normalized to the lower limit [cm³ water / cm³ soil]
τ	CO_2 use efficiency [m / s]
a	NO_x to nitrification proportion coefficient [-]
a_l	Empirical evaporation coefficient [-]
a_{DM}	Acidity modifying factor of decomposition [-]
$a_{DM,min}$	Acidity modifying factor reducing decomposition to a minimum [-]
ADS	Ammonium adsorption
adsc	Ammonium adsorption coefficient [-]
adsf	Empirical fitting constant regarding ammonium adsorption [-]
alb	Albedo
af	Nitrogen (ammonium or nitrate) availability coefficient for nitrogen root uptake [-]
amf	Ammonium limiting factor of related soil N processes [-]
AmMin	Minimum inert soil ammonium content [mg N / kg]
AP	Acidification potential [kg SO_2-equivalents]
ATT	Accumulated thermal time [degree days]
b_l	Empirical evaporation coefficient [-]
B:BH	Decomposition ratio of BIO to BIO+HUM pool
BD	Soil bulk density [g / cm³]
BD_{avg}	Average soil bulk density [g / cm³]
BIO	Microbiological SOM pool
biof	Soil microbial factor [-]
BM	Biomass
BPS	Biological production system
c	NO_x to nitrification proportion coefficient [-]
C	Carbon [kg C / ha]
$c_{1/2}$	Evapotranspiration coefficients as a function of crop type [-]
C_{Ia}	Initial abstraction ratio regarding runoff [-]
C_{IOM}	Amount of carbon in IOM pool [kg C /ha]
$C_{tot,meas}$	Measured total soil carbon [kg C / ha]
CAN	Calcium ammonium nitrate
cc_{DM}	Crop cover modifying factor of decomposition [-]
CC	Canopy cover
CEC	Cation exchange capacity [$cmol_c$ / kg]
CED	Cumulative energy demand [MJ-equivalents]
clay	Clay content [%]

$CN_{I/II/III}$	Curve number under dry/average/wet conditions [-]
C:N	Carbon to Nitrogen ratio [-]
CO_2	Ambient carbon dioxide concentration [µmol CO_2 m^{-3}air]
COB	Commercial crop yield [ton / ha]
crat	Decomposition ratio of CO_2 to BIO+HUM pools
CV_t	Coefficient of variation at time *t* [%]
DBAR	Water diffusivity [cm^2 / day]
DCB	Dichlorobenzene
DD	Damping depth [cm]
DD_{max}	Maximum damping depth [cm]
DENIT	Denitrification
dfs	Soil depth decomposition factor [-]
DM	Dry matter [g / plant]
DM_p	Daily plant dry matter increase [g DM / plant / day]
DM_X	Daily plant organ (X=leaf, stem or curd) dry matter increase [g DM / plant / day]
DPM	Decomposable plant material SOM pool
$DRAIN_l$	Saturated downward flow from layer *l* [cm]
DT	Change in soil surface temperature in time due to actual weather conditions [°C]
DVS	Crop developmental stage [-]
EF	Emission factor
EP	Eutrophication potential [kg PO_4-equivalents]
ESW	Extractable water available for diffusive flow [cm^3 water / cm^3 soil]
ET_0	Reference evapotranspiration for a grass surface [cm / day]
ET_c	Potential crop evapotranspiration [cm / day]
f	Half of the top layer thickness [cm]
F	Distance [cm] between the centres of the top layer and layer of interest
$F_{(D)N}$	*(De)n*itrification rate modifier due to environmental conditions [-]
fc	Amount of water between field capacity and lower limit [cm^3 / cm^3]
f_{ch}	Mineralisation correction factor [-] regarding clay and humus content (SALCA-NO_3)
f_{cr}	Mineralisation correction factor [-] regarding crop residue incorporation (SALCA-NO_3)
$f_{DM/(D)N/V}$	Rate modifying factor of decomposition/(de)nitrification/volatilisation of ammonia [-]
f_K	Evaporation crop coefficient decline factor [-]
F_l	Upward evaporation flow coefficient [-]
f_{risk}	Nitrogen leaching correction factor [-] due to fertilizer application (SALCA-NO_3)
f_{sd}	Nitrogen leaching correction factor [-] regarding soil depth (SALCA-NO_3)
f_V	Ammonia volatilisation rate modifier [-]
FC	Water content at field capacity [cm^3 water / cm^3 soil]
fert	Fertilizer

FF	Fractionated fertilizer application system -scenario
FFSC	Fractionated fertilizer application & soil cover system -scenario
$FLOWl_{,a/p}$	Actual/potential diffusivity flow from layer *l* [cm /day]
fN_p	Potential nitrogen limiting factor for soil decomposition [-]
FN_l	Nitrogen availability limiting factor for nitrogen root uptake [-]
FRUIT	Edible part of the crop, i.. the curd of cauliflower or shaft of leek
FU	Functional unit (of the life cycle assessment)
G	Soil heat flux density [MJ / m² / day]
GHG	Greenhouse gas
GRAD	Soil water content gradient [cm³ / cm³ /cm]
GREF	Growth efficiency [g DM / g CH_2O]
GWP	Global warming potential [kg CO_2-equivalents]
H	Hottest day of the year [Julianday]
HT	Human toxicity [kg 1,4-dichlorobenzene-equivalents]
HUM	Humus SOM pool
I	Intercepted water by the crop [cm / day]
I_a	Initial abstractions regarding runoff [cm]
Interc	Water interception by the crop
IOM	Inert organic matter pool
IPCC	International panel on climate change
Irrig	Irrigation
k	Interception correction factor for canopy throughfall [-]
$K_{C(,ini,max)}$	(Initial/maximum) evapotranspiration crop coefficient [-]
$K_{c,lai}$	K_c shape parameter as a function of LAI [-]
K_d	Dead leaf fraction coefficient [-]
k_H	Urea hydrolysis rate [/day]
$k_{j(=DPM/RPM/BIO/HUM)}$	Decay rate of a SOM pool *j (=DPM/RPM/BIO/HUM)* [/day]
K_{nh4}	Nitrification half saturation constant [mg N / L]
K_{no3}	Denitrification half saturation constant [mg N / L]
K_r	Evaporation crop coefficient water factor [-]
k_V	Ammonia volatilisation rate [/day]
KEP	Energy extinction evapotranspiration partitioning coefficient [-]
KNS	Kulturbegleitende N_{min} Sollwerte, i.e. fertilizer advisory system
LAI	Leaf area index [-]
LCA	Life cycle assessment
LCI	Life cycle inventory
LCIA	Life cycle impact assessment
Nleach	Nitrogen leaching
LL	Water content at lower limit [cm³ water / cm³ soil]
LT	Layer thickness [cm]
LO	Land occupation [ha]
$m_{0/1/2}$	Moisture rate modifiers at lower level / a threshold / saturation [-]
$m_{DM/(D)N/V}$	Moisture modifying factor of decomposition/(de)nitrification/volatilisation [-]
$MI_{(a/p)}$	Actual/potential mineralisation or immobilisation [kg N / ha / day]
N	Nitrogen [kg N / ha]

N_2	Dinitrogen [kg N / ha]
N_2O	Nitrous oxide [kg N / ha]
N_2O_{DN}	Emission of nitrous oxide due to denitrification [kg N / ha /day]
N_2O_N	Emission of nitrous oxide due to nitrification [kg N / ha /day]
N_{ADS}	Adsorbed ammonium [kg N / ha]
N_{CAN}	Nitrogen amount in CAN fertilizer
N_{cr}	Nitrogen from crop residues [kg N / ha]
$N_{dem,p}$	Potential N demand from the crop [g N / plant / day]
N_{DN}	Denitrified nitrate [kg N / ha / day]
N_f	Nitrogen from fertilizers [kg N / ha]
N_{fert}	Amount of monthly applied nitrogen fertilizer [kg N / ha] (SALCA-NO_3)
N_{min}	Monthly amount of mineralised nitrogen [kg N/ha] (SALCA-NO_3)
N_N	Nitrified ammonium [kg N / ha / day]
N_{upt}	Monthly nitrogen uptake (SALCA-NO_3)
N_X	N demand of plant organ X (leaf, stem, curd or root) [g N / plant / day]
NDAYS	Length of simulation [days]
NH_3	Ammonia [kg N / ha]
NH_4	Ammonium content [kg N / ha]
NH_4*	Ammonium content [mg N / kg]
nif	Nitrate limiting factor of related soil N processes [-]
NiMin	Minimum inert soil nitrate content [mg N / kg]
NIT	Nitrification
NLeach	Soil nitrogen leaching
NO_3	Nitrate content [kg N / ha]
NO_3^*	Nitrate content [mg N / kg]
NO_N	Emission of nitric oxide due to nitrification [kg N / ha /day]
NO_x	Nitric oxide [kg N / ha]
NSE	Nash-Sutcliffe modelling efficiency
NSTART	Start date of simulation
NUF	Nitrogen uptake factor [-]
OC	Organic carbon content [%]
P	Precipitation (including irrigation) [cm]
$P_{g(,h)}$	Gross (hourly) photosynthesis [µmol CO_2 / m² / s or g CH_2O / day]
P_{max}	Maximum leaf photosynthesis rate [(µmol CO_2 / m² / s]
P_{ni}	Net pecipitation (incl. Irrigation) excluding the intercepted water [cm]
Pbias	Percent modelling bias
PDR	Maximum potential denitrification rate [kg N / ha /day]
PDVS	Correction factor of leaf photosynthesis rate for leaf senescence [-]
Perc	Deep water percolation
PGRED	Correction factor of leaf photosynthesis rate for suboptimal temperatures [-]
PLD	Plant density [plants / m²]
PNR	Maximum potential nitrification rate [kg N / ha /day]
PPFD	Photosynthetic flux density or radiation intensity above the canopy [mol photons / m² /s]
$PT_{a/p}$	Actual/potential plant transpiration [cm / day]

$PVPD$	Correction factor of leaf photosynthesis rate for air vapour pressure deficit [-]
Q_e	Light use efficiency [µmol CO_2 / mol photon]
Q_{10}	Temperature effect coefficient maintenance respiration [-]
r	N_2O to denitrification proportion coefficient [-]
$r_{(D)N}$	(De)nitrification rate [/day]
$r_{di/le}$	Growth rates of shaft diameter/length of leek [cm / °C / day]
R	Release of CO_2 [kg C / ha / day]
R_m	Maintenance respiration [g CH_2O / d]
R_n	Net radiation at crop surface [MJ / m² / day]
R_{urea}	Release of CO_2 from urea [kg C / ha /day]
$RD_{(ini/max)}$	(Initial/maximum) rooting depth [cm]
RDM_l	Root dry matter in layer *l* [g / plant]
$RDPF(_{\sim}RD)$	Root distribution factor as a function of rooting depth [-]
$RedFac$	Soil evaporation reduction factor [-]
RefDate	Reference date for simulation
Rf_{sh}	Root to shoot ratio [-]
RH	Relative humidity [%]
RLD_l	Root length density in layer *l* [cm root / cm³ soil]
$RMR_{l/f}$	Respiration maintenance parameters of the plant organs [-]
RMSE	Root mean square error
$RNU(P)_l$	(Potential) root nitrogen uptake [kg N / ha /day]
RO	Runoff [cm]
RPM	Resistant plant material SOM pool
RSR	Root mean square error to observed standard deviation ratio
RTN_m	Maximum nitrogen uptake per unit root length [mg N / cm root / day]
$RTWU_m$	Maximum plant limited water uptake rate [cm³ / cm root / day]
$RWUP_{(m)l}$	(Maximum) potential root water uptake in layer *l* [cm³ water / cm root /day]
$RWU(PLa)_l$	(Potential) Root water uptake in layer *l* per unit area [cm / day]
S	Retention parameter regarding runoff [cm]
S_{rad}	Daily global radiation [MJ / m² / day]
S_t	Sensitivity of model output variable at time *t* to a parameter change [-]
sat	Amount of water between saturation and lower limit [cm³ / cm³]
SAT	Water content at saturation limit [cm³ water / cm³ soil]
SC	Soil cover system -scenario
SC_{max}	Maximum canopy storage capacity [cm]
sd	standard deviation
SDF	Soil deficiency factor [-]
$SE_{a/p}$	Actual/potential soil evaporation [cm / day]
$SE_{av,l}$	Available water for soil evaporation from layer *l* [cm / day]
$ShaftDi$	Shaft diameter of leek [cm]
$ShaftLe$	Shaft length of leek [cm]
$SMDFR_l$	Soil moisture limiting factor for nitrogen root uptake [-]
SLA	Specific leaf area [cm² / g]
Slp	Field slope [-]

SN_l	Soil nitrogen (ammonium or nitrate) concentration in layer *l* [mg N / kg]
SNDF	Soil nitrogen deficiency factor [-]
SolRad	Solar radiation [MJ / m²]
SO_2	Sulfur dioxide
SOM	Soil organic matter
SRL	Specific root length [cm / g]
SW	Total amount of soil water above lower limit [cm]
sw	Current amount of water above lower limit [cm³ / cm³]
SWDF	Soil water deficiency water [-]
SWEF	Soil water evaporation factor [-]
SWC	Soil water (or moisture) content [cm³ water / cm³ soil]
SWC_{eq}	Evaporation threshold water content [cm³ / cm³]
SWC_{tot}	Total amount of soil water [cm]
$swcon_{1/3}$	Empirical water uptake resistance constants [-]
$swcon_2$	Water uptake constant as a function of the lower limit [-]
$SWCON_l$	Soil water conductivity or drainage rate constant [/day]
SWLeach	Soil water leaching
$t_{DM/(D)N/V}$	Temperature modifying factor of decomposition/(de)nitrification/volatilisation [-]
T_a	Mean daily air temperature [°C]
T_b	Crop growth base temperature [°C]
T_{amp}	Monthly air temperature amplitude [°C]
T_{ef}	Effective temperature, i.e. air temperature corrected for base crop growth temperature [°C]
T_m	Mean air temperature [°C]
T_{max}	Maximum air temperature [°C]
T_{mod}	Optimal soil temperature for ammonia volatilisation [°C]
T_{ref}	Respiration reference temperature [°C]
T_s	Soil temperature [°C]
$T_{s,a}$	Five-day moving average of the actual surface soil temperature [°C]
T_{surf}	Soil surface temperature [°C]
$TDM_{(G)L/S/C}$	Total dry matter of a plant organ (=(green) leaf, stem or curd) [g DM / plant]
TDR	Time domain reflectometry (sensor)
Temp	Temperature
TH	Water content at a threshold [cm³ water / cm³ soil]
TotLeafArea	Total leaf area [m² leaf / g leaf DM]
u_2	Wind speed at 2m height [m / s]
UPT	Uptake
VOL	Ammonia volatilisation
VPD	Vapour pressure deficit [kPa]
$w_{1/2}$	Shape coefficient regarding runoff retention parameters [-]
W	Gravimetric water content (g water / g soil]
$W_{d,l}$	Oversaturated downward flow from layer *l* [cm]
$W_{N,l}$	Amount of nitrogen (ammonium or nitrate) drained from layer *l* [kg N / ha]

$W'_{N,l}$	Amount of nitrogen (ammonium or nitrate) diffused from or to layer *l* [kg N / ha]
$W_{p,l}$	Potential downward flow from layer *l* [cm]
WC_r	Relative water content [-]
WFPS	Water filled pore space [- or %]
WUF	Water uptake factor [-]
X_f	Dry matter fraction of a plant organ [-]
X_K	Light extinction coefficient in the canopy [-]
X_M	Light transmission coefficient in the canopy [-]
X_{Nc}	Critical N concentration of a plant organ X (leaf, stem, curd or root) [-]
z	Depth of soil layer [cm]
z_{DM}	Depth modifying factor of decomposition [-]
$Z_{c,l}$	Water (and nitrogen) fraction of layer *l* diffused [-]
$Z_{p,l}$	Water (and nitrogen) fraction of layer *l* drained [-]

Table of contents

Chapter 1. General introduction and objectives

Climate change, rising energy use and other environmental threats have become more and more pressing, and there is emerging socio- political consensus that action is urgently needed. Mobility (automobile and air transport), food (meat, poultry, fish, dairy and plant-based), and residential energy use in the house (heating, cooling, electrical appliances, and lighting) are responsible for the largest share of environmental impact (Brouwers et al., 2017; Tukker and Jansen, 2006). Partially these sectors involve biological systems that are often complex and difficult to control and measure. Agriculture, fundamental for human well-being, is a major cause of environmental decline (Foley et al., 2011; Johnson and Villumsen, 2018) and thereby the key to attaining the UN Sustainable Development Goals of eradicating hunger and securing food for a growing world population of 9-10 billion by 2050 in a world of rising global environmental risks (Godfray et al., 2010; Rockström et al., 2017). Assessing the environmental impact of related products, let alone its sustainability, is a difficult task but also an emerging research field. A wide range of methodologies have been proposed, from indicators (e.g. carbon footprint) to product related assessments (e.g. life cycle assessment) and integrated assessments (e.g. multi-criteria analysis) (Ness et al., 2007; Suopajärvi, 2011). As we are evolving towards a green economy, there is a need to implement these methodologies in decision making and system management in every sector (Bausch et al., 2014; Valdivia et al., 2013). Furthermore, the present organisation of our food production leads to significant alterations of the global nitrogen (N) cycle which is an important cause of increasing nitrogen emissions into ecosystems and the atmosphere (Sonesson et al., 2010; Zhang et al., 2015). Aiming at sustainable systems requires to account for long-term implications of practices and the broad interactions and dynamics of agricultural processes. A key goal hereby is to understand agriculture from a biophysical perspective in terms of water and nutrient dynamics, and interactions between plant and soil under changing climate conditions. An holistic modelling framework is thereby recommended to represent the farming system and support its sustainability assessment as mentioned above (Kersebaum et al., 2004; Le Gal et al., 2010; Wei et al., 2009). Such approaches furthermore deal with sensitivity and uncertainty of the input and the impact results as well for instance due to either the modelling approach and/or the management and inherent climate variability (Guo et al., 2012).

1.1 Technical sustainability in agriculture

With the world's movement towards sustainable development, also agriculture faces mounting pressure to reduce its environmental impact. With an increasing world population, it is certainly a challenge as the agricultural sector is forced to increase productivity, provide various vital ecosystem services and reduce costs while maintaining product quality and respond to regulatory and market shifts

(Bennett et al., 2014; FAO, 2013; Rockström et al., 2017; Valdivia et al., 2013). It is believed that knowledge, technical competence, and skilled labour needed to manage the agro-ecosystems effectively are crucial towards sustainability. In order to assess sustainability, many definitions and tools have been proposed. Although it is still subject to discussion, most definitions encompass the ideals of economic profitability, environmental health and social equity. As starting point, often is referred to the Brundtland Commission: ‘sustainable development is development that meets the needs of the present without comprising the ability of future generations to meet their own needs’ (United Nations, 1987).

Sustainability has become one of the major topics of interest in farming systems research. Several approaches and methodologies have been proposed and developed revolving around the three commonly accepted pillars of sustainability (i.e. economic, social and environmental) (Hayati et al., 2010; Ness et al., 2007; Van Cauwenbergh et al., 2007). Reports describe economic (e.g. food prices, subsidies,...), social (e.g. food security, labour conditions,...) and environmental risks (e.g. resource depletion, increasing greenhouse gasses,...) within the agricultural system.

Given the definition of (agricultural) sustainability, the present work intends to evaluate the sustainability of a biological production system (BPS) by addressing the technical aspect prior to the other three. Technical sustainability is defined as the ability of a BPS to make an efficient use of the available resources with the main goal to maximize its economic output given a set of uncontrolled biophysical constraints (Bojacá et al., 2012). The biophysical environment in which the agricultural processes take place consists of series of interactions and relationships that limit the ability of the system to reach its maximum sustainability on every level. Moreover, temporal and spatial variability, inherent to any biological production system, impede the efficiency. The definition of technical sustainability covers also the environmental dimension. Efficient use of water and nutrients is required through an optimal fertilizer management as a function of the crop development and weather to achieve maximum uptake by the plant avoiding or limiting the potential losses of nutrients to the environment through runoff, leaching or air emissions. Once the management practices are optimised to attempt to control these natural processes, only then can the maximum yield be achieved, although external factors like extreme weather events or pests and diseases might decrease the expected production.

1.2 Biological production systems

The technical sustainability of a biological production system within this dissertation was assessed on the level of the production field where complex interactions between inputs (e.g. inorganic fertilizer) and outputs (e.g. food) and between basic natural processes (e.g. nutrient uptake) and unit operations (e.g. fertilizer application) take place. It is presented in Figure 1-1 that, although not complete, serves as a reference. The technical sustainability at the production field focuses on the efficient use of inputs within the boundaries of the system while economic and social issues are considered as externalities of the production process belonging to higher levels of aggregation as the farm or community. The higher level might be chosen as unit for example in animal production. With advances in science and growing needs in the society the biological systems function can be expanded from production of food, over fibre to fuel and fine chemicals. Nevertheless, the main emphasis in this work is set on crop production, the soil processes and the environmental impact that it brings along. Both the basic natural processes addressed by the modelling (see section 1.4 and Chapter 4), and the environmental impact quantified by the life cycle assessment (see paragraph 1.3, Chapter 3 & Chapter 7) fall back on this systems approach.

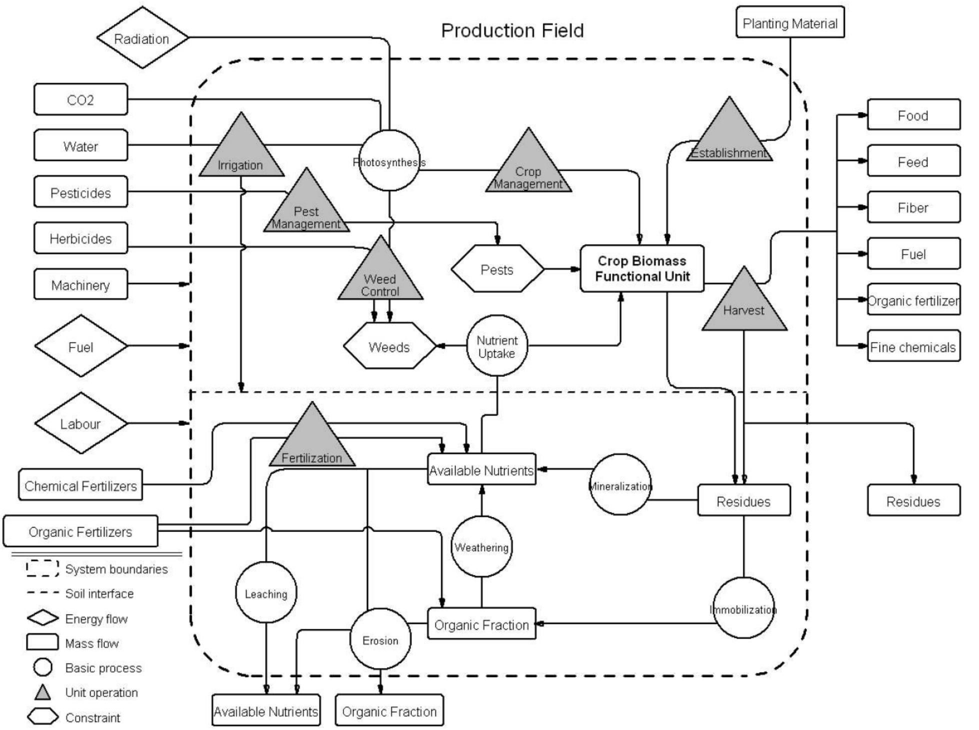

Figure 1-1 Flow diagram of a biological production system identifying system boundaries at field level, mass and energy flows, basic processes, unit operations and selected constraints (Bojacá, 2009)

1.2.1 Impact of horticulture in Flanders, Belgium

Although horticulture in Flanders covers only 7.5% of the agricultural area (45548 ha in 2015), with an end production value of 1.1 billion Euros, it represents 20% of the total agricultural production in 2015. Vegetable production generates up to 42% of the end production value of the total horticultural activity. Furthermore, about 96% of the cultivated area is destined for open field production, of which 55.7% is occupied by vegetables with leek, cauliflower and endives as the most prominent ones (Platteau et al., 2016). This explains the pressure on the limited production area which has encouraged farmers to excessive use of relative cheaper inputs as fertilizers, pesticides and energy. Also the lack of regulation regarding the impact and/or the corresponding environmental costs, does not stimulate more efficient production with less impact. Furthermore, agricultural production is economical fragile due to volatile input prices, insecure product prices and the cut-off of large export markets due to geopolitical problems (Brouwers et al., 2017).

Efforts to decrease emissions of agriculture have reduced the environmental impact from 1990 till 2008 in general, but they seemed to have stagnated since. The share of agriculture in the total Flemish greenhouse gas emissions reached 10% in 2011 as agriculture released 53% of total nitrous oxide due to soil denitrification and 76% of total methane (Platteau et al., 2014), with animal husbandry and arable farming the main contributors. Acidifying emissions originate for 41% from agriculture mainly because of ammonia from animal manure and synthetic fertilizers (81%) and nitric oxide from the soil after fertilizer applications (13%). Due to additional losses of nitrogen through leaching, agriculture represents 50% of total nitrogen losses in Flanders while residences, trade and services comprise 30% together due to fossil fuel incineration (Brouwers et al., 2017).

1.2.2 Nitrogen fertilizer management

Mankind has sought for different ways to increase the crop production necessary to feed a growing population. This has led among others to the development of synthetic fertilizers and further intensification of agriculture. These developments raise the question to what extent this and/or other technologies affect the sustainability of the production systems. In 2014 the total synthetic N fertilizer use in Flemish agriculture raised up to 78.4 million kg N, with an average of 110 kg N/ha. For leek, the rate amounted up to 147 kg N/ha (Lenders and Deuninck, 2016). Inefficient use of plant nutrients puts agriculture as the largest contributor to Europe's freshwater pollution by 50-80 % of the total nitrogen load (EEA, 2010). Despite some efforts during the last two decades to reduce nutrient input and losses, the eutrophication pressure from agriculture in absolute values remains at a high level (Van Steertegem, 2013). While the application of N containing fertilizers and manure is essential, excessive use constitutes an environmental risk. To protect the vulnerable natural environment against pollution caused or induced by nitrate (NO_3^-) leaching from agricultural sources, the European Nitrates Directive (91/676/EEC) has imposed a maximum concentration level of 50 mg NO_3^-/L in groundwater and surface waters in accordance with the quality standard for potable water (Anonymous, 1991). Data from the water monitoring network of the Manure Action Plan (MAP) of Flanders reports that still 21% of the sampling points exceeded the threshold in the winter of 2013-2014 which was above the projected 16% and still far from the 5% target in 2018 (VMM, 2016). Vegetable production, known for the large amount of fertilizer applications, is the largest contributor to nitrate residues in the soil, with cauliflower and leek as a common crop rotation in the top three (VLM, 2008). As an additional measure to reach the targets stated, the N surplus on the soil balance is set at 70 to 90 kg N/ha stipulated by the Flemish environmental policy in a 5 year MINA-plan. The actual threshold depends on cultivation, soil type and the location in 'focus areas' due to threshold exceedance and/or insufficient progress in the past (Heirman, 2011; VLM, 2015).

Available advisory structures regarding fertilizer management are divided in three main types (Geypens and Vandendriessche, 1996):

1. based on soil analysis (e.g. N-index method by the Soil service of Belgium or Kulturbegleitende N_{min} Sollwerte system (Lorenz et al., 1985)): no feedback of plant requirements in correspondence with the prevailing weather is incorporated nor the information on soil type, its drain characteristics and nutrient dynamics.
2. based on plant analysis (e.g. Sensor based nitrogen rate calculator SBNRC; (Butchee et al., 2011)): requires detailed calibration and lacks incorporation of important soil processes and crop residue incorporation.
3. based on simulation models (CropSyst (Stockle et al., 2003), DSSAT (Jones et al., 2003); EU-Rotate_N (Rahn et al., 2010); NDICEA (Van Der Burgt et al., 2006); STICS (Brisson et al., 2003) or WAVE (Vanclooster et al., 1996): predict the nitrogen dynamics in plant or soil or combined (see further paragraph 1.4).

Thus, converting to sustainable practices does not mean simple input substitution. To develop efficient biological systems and ensure long-term productivity and stability, enhanced management and scientific knowledge is required. The challenge is still to better understand the extent of nitrogen enrichment regarding fertilizer application, plant and soil processes under changing climate conditions and to evaluate their respective impact on the environment (Erisman et al., 2011). In Flanders, climate change would mainly manifest itself in a strong increase of temperature with more frequent hottest days and in a larger precipitation variability with an increase of especially winter rainfall. A higher risk of water stress is expected with fluctuations in yield (Brouwers et al., 2017).

1.3 Life cycle assessment

Life cycle assessment (LCA) was initially developed to evaluate the environmental impact of industrial products and processes. LCA is defined by the International Organisation for Standardisation (ISO 14040:2006) as "the compilation and evaluation of the inputs, outputs and potential environmental impacts of a product system throughout its life cycle" (Guinee et al. 2002). It has become a widely recognized method within the sustainability assessment for quantifying the environmental performances of products. The environmental burden covers all types of impacts, including extraction of different types of resources, energy use, emission of hazardous substances and land use. LCA provides a comprehensive and objective method of analysis that identifies the

environmentally most dominant stage in a product life cycle where major consumption of resources and emissions to the environment occur and hence indicates the “bottlenecks” to be improved. It also allows the comparison of alternative production systems. Based on this analysis, policy makers are able to determine the environmental profile of a product (or service). LCA supports them in strategic decision making regarding optimisation of the system, adaptation to environmental changes and more severe constraints, etc.
The literature is diverse in its goals, methodologies and coverage of industrial and even agricultural products (Finnveden et al., 2009; Harris and Narayanaswamy, 2009; Hayashi et al., 2006; Roy et al., 2009; Williams et al., 2006). Applying an LCA to agricultural systems requires consideration of its complex interactions and dynamic nature as mentioned above. Farms have a large variability in both natural factors (climate, soil etc.) and management factors (farm size, cropping management etc.), and through difficult-to-measure emissions (Nemecek and Erzinger, 2005; Perrin et al., 2014). Functional principles of agricultural systems are quite well understood, but not all underlying material flows can be easily quantified. It is essential to find an appropriate assessment with system boundaries equally valid, both in agricultural practice and in the LCA model. This is relevant, because the quality of this representation affects the quality and meaningfulness of the overall LCA results. Although LCA is praised for its holistic approach, it has an inherent static nature and heavily depends on the quality of input data. Recent review study by Notarnicola et al. (2017) confirms the need for dedicated modelling approaches due to the intrinsic variability of food production systems although it refers to the standard empirical approaches (addressed in the next section) and mentions the lack of consensus on a globally applicable model for calculating soil and water emissions which are more dependent on soil conditions.

1.4 Modelling

Although field emissions due to fertilizer application and several soil processes can contribute considerable to the impact of the food product, they are often disregarded in studies. Estimating field emissions in agricultural LCA’s poses major problems as these emissions are highly variable due to the crop, soil, climate and management interaction (Bessou et al., 2012).
If they are accounted for, different calculation pathways (or Tiers) are applied, characterized by a different degree of complexity and mathematical description of the processes involved (IPCC, 2006). The most common practice is using Tier 1 methodologies, which are however intended for use at large spatial scales and can generate substantial errors in predictions at finer scales, mostly due to different soil, climate and management practices. Higher Tiers 2 & 3 are usually considered too complex and time consuming to be tractable in the development of LCA studies. The huge amount of data required (meteorological data, crop phenological data and chemical and physical soil characteristics) to run these models and establish the LCA inventory could limit widespread use of this

approach (Bosco et al., 2013). This leads also to more balanced approaches through combinations (Williams et al., 2010). For example, Bouwman et al. (2002a, 2002b) summarized and modelled the results from 846 and 99 studies detailing respectively nitrous and nitric oxide emissions from farmland. These studies are predominantly based on measurements taken in gas collection chambers placed out on fields. Both created model estimated emissions from factors including fertilizer rate and type, crop type, soil texture, pH and soil carbon content, drainage and climate.

Widely applied in LCA studies, empirical models address field emissions as provided by Nemecek and Schnetzer (2012) which mainly consists of Tier 1 functions like IPCC guidelines (IPCC, 2006) and the Tier 2 approach for nitrate leaching by the SALCA-model (Richner et al., 2014). They imply nitrogen flows proportional to the supply of fertilizers and a limited variation in the regional agro-ecosystem. The dynamic nitrogen processes however are tightly linked to climate conditions, soil properties and crop characteristics. There is an urgent need for the application and validation of appropriate higher tier methodologies at farm, project, or plantation scales, to address local issues with food sustainability and identify local mitigation potentials (Cannavo et al., 2008; Peter et al., 2016). Therefore more site-specific process-oriented models (Tier 3) are developed to address the interactions including microbial, plant physiological and physicochemical processes affected by environmental conditions (Guo et al., 2012; Vogeler et al., 2012). Agro-ecosystem models are more and more applied to support decision-making at different scales, ranging from fertilizer recommendations for farms on a field scale up to a landscape or regional scale for strategic policy decision support (Kersebaum et al., 2004). Input data are becoming scarce and uncertain and meanwhile data of relevant state variables for calibration are not available. This requires robust models, which are able to generate their input requirements from basic standardized soil data without the necessity of parameter calibration. On the other hand, model users and decision-makers expect that the validity of models used has been proved comparing uncalibrated modelling results with field observations outside the range of model development. The large spatial and temporal variability of soil mineral nitrogen and the multiple processes and interactions influencing the soil nitrogen dynamic make it however difficult to achieve good agreements and still seem to be a challenge for models (Kersebaum et al., 2004).

Although modelling of soil carbon and nitrogen dynamics has been in the literature since the 1960s, it is still one of the least understood areas. The modelling concepts originate from chemistry and biology and are applied to agricultural sciences without considering the limitations of many of the theories. Many of the process rate equations apply only to ideal solutions or populations, which seldom exist in the heterogeneous soil environment (Shaffer et al., 2001b).

Various models have been elaborated that differ according to

1. the processes accounted for: typical crop models (e.g. SUCROS (Van Laar et al., 1997)), soil models (DAISY (Abrahamsen and Hansen, 2000)) or gas

emission models (NOE, (Henault et al., 2005)) imply simplification for the respective other processes. Integrated models do intend to account for all main processes (e.g. DSSAT-CSM, (Hoogenboom et al., 2015), APSIM (Keating et al., 2003), CERES (Jones and Kiniry, 1986)) which are mostly based on the single models and also show overlap for some processes.

2. the type of equations used: there has been a shift from mechanistic to functional models involving more simplistic approaches due to limited access to data and aggregation of modules according to specific objectives which impede extrapolation to other pedo-climatic and crop contexts and/or access to the details of these modifications. It shows there is a need for modular systems with modules describing various processes with various level of complexity. Accordingly, alternatives should be addressed to overcome the limited conditions under which the applied processes are valid.
3. the time and space scales: regarding time, the most commonly applied time step is the daily step compared to a monthly step (CENTURY (Parton et al., 1993)) or to a crop cycle aggregation (INDIGO-PERSYST (Bockstaller and Girardin, 2003)). Thereby, field scale has been the most often represented compared to watershed (SWAT (Neitsch et al., 2011)) and farm scale (FARMN (Jorgensen et al., 2005)).
4. the extent of calibration and/or validation which relates to the input data and their degree of accessibility: lack of model testing at field scale.
5. the model performance: only few papers show comparisons between model simulations and field measurements while most are purely restricted to simulations and scenario tests, so they lack statistical outcome or are limited to data visualisation.

The rotation scale is the relevant one for assessing the impacts of changes in cropping systems. Predicting N losses accurately needs N partitioning between shoots and roots, as well as root characteristics. On this timescale, the impact of the parameters of a single crop on the model outputs is smoothed. Moreover, extending the temporal boundary to a rotation cycle overcomes difficulties of attributing the effects of unit operations to single crops within the context of a LCA. Farmers optimize their production for a whole crop rotation, which could also imply the reduction of impacts that occur at a different timing than the moment of operation that causes them (Nemecek et al., 2001).

Finally, it has been shown that when building models to be used in different contexts, it is necessary to test the sensitivity of the model over a wide range of diverse databases, and to elaborate correction functions taken into account the main explanatory factors of a process. It will serve as a more profound basis to conduct further improvements and implementation of the model on various case studies or future perspectives (Cannavo et al., 2008; Constantin et al., 2012; Thorp et al., 2014). Furthermore, this helps in subsequently addressing the uncertainties due to model parameters and model structure and uncertainties inherent to dynamic systems due to for instance climate variability or soil properties (Monod et al., 2006; Payraudeau, 2007).

1.5 Objectives

In general, this research aims at assessing the technical sustainability of a biological production system. Gaining insight in the nitrogen dynamics in a crop-soil system that is affected by the weather and by nitrogen fertilizer management, should improve the evaluation of their impact on the nitrogen flow within the system and towards the environment. It is hypothesised that the integrated dynamic model based life cycle assessment provides a more reliable and realistic evaluation of the environmental impact and technical sustainability of a biological production system. To meet this overall objective and evaluate the hypothesis, the following queries were addressed along the associated research questions:

What is a commonly applied method to evaluate the environmental impact of a crop rotation system? What are the bottlenecks? What are the effects of different N dose rates over multiple years with varying weather?

- → Default life cycle assessment of the system with an empirical estimation approach regarding nitrogen field emissions

How does the crop growth integrate with soil water and nitrogen dynamics affected by varying weather and different fertilizer application rates?

- → Development of an integrated dynamic crop-soil model at field scale

How is the model (performance) evaluated and optimized to address different conditions?

- → Calibration and validation of the model under different N rates over multiple years with experimental observations

To what extent does the model enhance the environmental impact assessment and does the integrated approach contribute to the technical sustainability evaluation? What are the implications of future management?

- → Implementation of the dynamic model to support the default life cycle assessment and to run a scenario analysis involving potential impact reduction strategies

More specifically, the open field production of a cauliflower leek rotation in Flanders, Belgium was chosen as case study throughout the whole research. It is a commonly applied rotation cycle susceptible for excessive use of inorganic nitrogen fertilizers.

1.6 Originality and outline of the work

Within the scope of environmental impact assessment in agricultural systems research, several aspects of this work can be considered innovative.
The study applies in first instance the widely used life cycle assessment with standard procedures to address the environmental impact on the field production stage from ‘cradle-to-gate’ like many previous studies as reviewed by Perrin et al.

(2014). Although, some still lack (transparency of) adequate estimations of field N emissions (Peter et al., 2016). As a first approach, a default LCA was applied to a nitrogen fertilizer management during a yearly rotation cycle of cauliflower and leek, used as a case study throughout the entire study. The data collection itself was also a particular challenge regarding the experimental setup and gathering representative data from frequent periodical destructive sampling and image analysis to root mass estimation. For three consecutive years, data was collected and analysed through consistent sampling and monitoring of mainly crop growth, soil temperature, soil water and nitrogen content under different fertilizer application rates given the following model development, calibration and validation. The data acquisition was the joint responsibility of

Furthermore, the impact assessment procedure is written in R (R Development Core Team, 2015) which allows fast and flexible impact quantification and visualisation of multiple crop rotations, even within the same year, while this is less feasible with available commercial LCA software. Also, two functional units of kg commercial yield and kg 'edible' yield were used to account for nutrient 'allocation efficiency' and the food waste aspect in relation to the environmental impact.

To overcome the drawbacks of the by default static LCA outcome and provide reliable field nitrogen emission data, an integrated model is entirely developed in R as well. Crop- soil modelling contributes to the development of innovative management strategies. It is becoming a valuable tool for increasing our understanding and sustainable agricultural production under a continuously changing climate, as it expresses the response of living system components to their physical, chemical and biological environmental conditions in a dynamic way (Ahmed et al., 2013; Wallach et al., 2014). A hybrid model is developed, incorporating existing and (still) up-to-date dynamic and process based models that attempt to be mechanistic, based on scientific principles, rather than empirical, in order to be as generic as possible. However, a hybrid structure is inevitable, as "mechanistic" models contain functional or empirical components, especially when applied to biological systems. The model selection also took into account the applicability of a certain submodel in current studies to allow future comparison of the results. This work rather preferred to focus on the dynamic characteristic of the system model as the timing of natural processes or management is of importance. The key challenges comprised (i) selecting appropriate submodels applicable to a broad range of environmental conditions, (ii) translation of model equations and especially model concepts in simulation coding, (iii) integrating the different submodels implementing availability limiting factors and a feedback loop if stress conditions should occur and (iv) calibrating the entire model for the selected case study with the available data. The final model based LCA ultimately allows decision-making that goes beyond the evaluation performance of a default LCA.

The work further intends to serve as a manual or guideline useful for implementation in other site-specific studies as the proposed system model attempts to be applicable to any kind of farming system with different horticultural crops and different environmental soil and weather conditions.

This dissertation consists of 7 chapters after the present introduction sketching the issues around N dynamics in a crop-soil system and the need to evaluate the impact through an integrated modelling approach (Figure 1-2).

- **Chapter 2** describes the experimental setup and techniques used for acquiring the field data that is been used in the life cycle assessment and for model calibration and validation.
- A default life cycle assessment of the case study with an empirical approach to assess the nitrogen flows is performed in **Chapter 3**.
- **Chapter 4** is the description of the integrated model developed to simulate the nitrogen dynamics in a crop-soil system.
- **Chapter 5** deals with the model calibration with data from the experiment and the model response to parameter changes through a local sensitivity analysis.
- The model performance is validated in **Chapter 6** under different nitrogen dose rates and changing conditions of subsequent years.
- Ultimately the model is implemented in the LCA in **Chapter 7** and compared with the default one.
- **Chapter 8** closes the research work with overall conclusions and perspectives for future work.

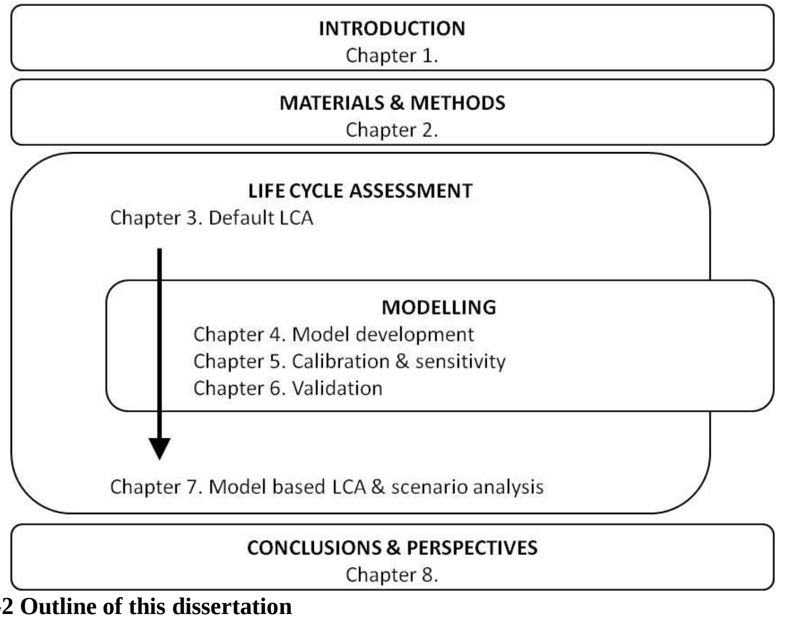

Figure 1-2 Outline of this dissertation

Chapter 2. Experimental setup and data acquisition

As part of the IWT funded research project *EcoFert* (On-line monitoring and model based decision support system for a 'just-on-time' nitrogen fertilisation in open field vegetable production), the experimental data used in this work was gathered over a period of 3 year starting at the planting of cauliflower in March 2009. The data acquisition was the joint responsibility of PhD students Joachim Vansteenkiste (eg. Vansteenkiste et al., 2014), Jelle Van Loon (Van Loon et al., 2011) and Reindert Heuts (this work and cf. 'List of publications' section). The experimental setup, the various methods for data acquisition and the sampling schedules during the experimental period will be described below.
Non-destructive as well as destructive plant and soil samples, leaching water samples and climate data were collected on a regular basis from the experimental field installed in the experimental research centre for vegetable production in Sint-Katelijne-Waver, Flanders (PSKW, or '*Proefstation voor de groenteteelt'*). Furthermore, several data collection methods were developed, tested and fine-tuned for this study.

2.1 Experimental setup

2.1.1 Setup

At the research centre 32 arable beds of 40m long and 1.4m wide were prepared as experimental units. Each of these plots was provided with an impermeable foil at a depth of 90cm over half their length resulting in a subplot with and without foil underneath. At the subplot borders, the foil was extended upwards in order to form a container that collects all the water that drains out of the root zone. Within these foil containers a drainage pipe was placed at the bottom, collecting the percolate into a separate 1 m³ barrel through a pumping system. As such, the quantity of drained water per (sub)plot could be measured through a height sensor in the collection barrel and analysed for mineral nitrogen (N) content. Furthermore, each subplot unit was equipped with a number of sensors for continuous online monitoring of the soil moisture content and temperature. Meanwhile weather data including precipitation, air temperature, solar radiation, humidity and wind speed, was collected on hourly basis. Every day all this data was wired to a server, ready for analysis. An overview of the installation is presented in Figure 2-1 and Figure 2-2 .

Figure 2-1 Overview of the experimental setup. From top to bottom, from left to right: i) aerial view of the Experimental station in Sint-Katelijne-Waver, Flanders and the experimental field (req square), ii) each subplot is contained in an impermeable foil, iii) collection of leaching water, iv) soil moisture and temperature sensors, and v) the experimental field, covered by leek.

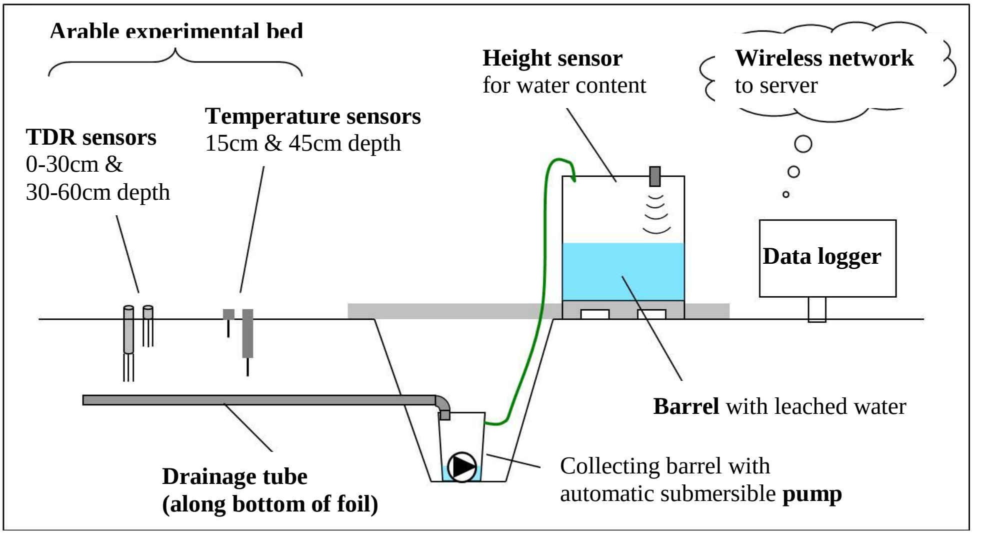

Figure 2-2 Schematic representation of the monitoring installation for each experimental plot

Every year a cauliflower- leek rotation was maintained. Cauliflower was planted in spring with a density of 4 plants m^{-2}, usually at the beginning of March and harvested in May/June after around 90 days. Subsequently, crop residues were incorporated into the soil and leek was planted, with a density of 18.18 plants m^{-2}, at the end of June to be harvested around 140 days later at the start of November. During the winter period the experimental plots remained untouched.

The experimental plots were grouped into two blocks of 16 plots which were treated every growing season with four different nitrogen application rates (or N doses), combined with four different nitrogen application treatments (broadcast, row application, fertigation and row application with a nitrification blocker), thus constituting a full-factorial trial (4×4 levels) replicated in two randomized complete blocks. In this thesis only the broadcast application of N fertilizer is discussed. The same treatment was applied on the adjacent undisrupted subplots which were not contained by a foil.

The amount of nitrogen applied with each dose, altered over the years. The differences in N levels were increased in order to find potentially more significant differences in plant nutrient availability levels. The lowest dose (N dose 1) was purposely chosen to create a nitrogen deficit. The last year in 2011, this dose was even set to zero, forcing the plant to grow on merely soil residual nitrogen. The highest dose (N dose 4) was chosen to establish a situation of luxury consumption by the crop. N dose 3, also referred to as reference (N) dose, was the advised dose recommended by the *Kulturbegleitende* N_{min} *Sollwerte* (KNS)-system developed in Germany (Lorenz et al., 1985), assumed to be optimal for photosynthetic capacity. The second dose (N dose 2) fell within rates 1 and 3 according to an equidistant interval. More detailed information is also presented in Chapter 3.

The application strategy, used in this work, was a commonly used broadcast system by a tractor with calcium ammonium nitrate (CAN). For cauliflower, the

N fertilizer was applied twice in the growing period, once at the planting and again 7 weeks after. As the crop residues of the cauliflower crop were incorporated before the start of the leek cultivation, representing a nutrient supply, the mineral N fertilizer application in the subsequent leek crop occurred 5 weeks after planting the leek. Every time the N fertilizer rate levels were essentially the target values for the mineral nitrogen in the soil: The actual quantity of N applied on the plot was calculated as the target N value minus the amount of mineral nitrogen present in the soil, determined through soil sample analysis prior to the fertilizer N application.

2.2 Data acquisition methods

To acquire the necessary data various techniques were used regarding weather, soil and crop related characteristics.

2.2.1 Weather data

Two different measuring systems compiled the weather dataset. The KMI Meteorological Station (from the Belgian Royal Meteorological Institute or '*Koninklijk Meteorologisch Instituut'*), installed at the experimental site registered on hourly basis the regular weather data, like sun radiation, temperature and relative humidity. Precipitation data was collected by a HOBO Data logging Rain Gauge–RG3M, a tipping bucket measuring system, also installed at PSKW, through which cumulative amounts of rainfall were logged. Additional historical weather data was extracted from data provided by the KMI.

2.2.2 Soil and solute related data

Besides measuring climate, the soil was monitored either continuously through sensors regarding the soil water content and temperature, or through discrete sampling and analysis for its nitrogen content.

Soil sensors

Over two depths from the surface of 0-30cm and 30-60cm a 30-cm long Time Domain Reflectometry sensor (TDR) was installed vertically at each field plot measuring the soil moisture content (volume % or cm^3 water cm^{-3} soil) which is negatively correlated with the velocity by which electrical pulses travel along the probe in the soil layer (Evett, 2003). Hourly measurements were registered at a data logger along with two temperature measurements through sensors at the depths of 15cm and 45cm.

Soil samples

A specific soil sampling routine was developed taken into account different positions in the plot relative to the rows and the plants within the plot. In total 6 spots for cauliflower and 4 for leek comprised samples at the plant and between the plant rows and within (not for leek due to larger plant density). According to this sampling template (Figure 2-3), representative samples of the 0-30cm and 30-

60cm soil layers were collected on regular times during the growing season to follow up the soil N status. Also, at planting and after 5 or 7 weeks depending of the crop, this allowed the estimation of the fertilizer amount to be applied to reach the target value (see above).

Figure 2-3 Unique soil sampling spots: 6 for cauliflower plots (upper) and 4 for the leek (lower).

The actual mineral nitrogen analysis of these samples was a combination of an extraction with a molar potassium chloride solution and a subsequent determination of the nitrate and ammonium by spectrophotometry (EMIS, 2010).
As mentioned above, the drained or leached water was collected into barrels. On regular basis they were emptied and samples were analysed for their nitrogen content at the same way as the soil samples. Unfortunately, the outcome of leaching measurements seemed highly variable and thus was only used as an indication rather than they were actually used for calibration or validation.

2.2.3 Crop related data

Destructive as well as non-destructive measurements were carried out at regular intervals during the growing season to collect crop related data. Destructive measurements consisted of biomass samples and corresponding nitrogen content analysis for the various plant organs. The non-destructive measurements included the leaf area index and the canopy cover. Finally, the rooting system, which affects the plant nutrient uptake from the soil, was investigated in more detail for both crops in 2011.

Biomass samples

Besides the initial characteristics of the seedlings at the start, biomass concerning fresh and dry weight was recorded four times during the growing season and with the harvest. At the latter also the separate weight of the plant organs (leaf and stem, and curd in case of cauliflower) was registered, with additional measurements of the shaft length and diameter with the leek crop. Every time samples were taken from 10 cauliflower plants or 24 leek plants per subplot (with and without foil underneath). In contrast to cauliflower which undergoes a change in phenology (i.e. curd initiation) during its growth, it is the stem or shaft of the leek which evolves to a mature 'fruit' to be consumed. Commercially sold cauliflower includes a leaf-stem crown attached to the curd. Furthermore, samples of the cauliflower residues, i.e. the leaves that stay on the field, cut off from the whole crop, were analysed.

Additionally the weight and surface of every leaf from a random selection of plants were determined. A LICOR LI-30000 Portable Leaf Area Meter obtained the leaf area for leek plants while for cauliflower, as its leaves were too big nor flat, a picture of the separate leaves per plant was taken to calculate the area through an image analysis. The leaf area index (LAI, m^2 leaf m^{-2} soil), i.e. the total leaf area per m^2 soil, was directly derived with the plant density. The ratio of leaf area to its weight determined the specific leaf area (SLA, $cm^2\ g^{-1}$) which in turn was used to simulate the leaf area from the predicted leaf biomass in the model.

At the same time the fraction of stem to leaf on plant fresh weight was recorded to better understand the plant biomass compartmentation.

In 2011, fewer recordings over time and per plot were carried out due to labour intensity, reducing for example the dry weight measurements from plant to plot level.

A Mettler Toledo PB602-S precision balance was used to weigh all the fresh samples and after a period of minimum 10 days in an industrial oven at 70°C, the dry samples as well.

Nitrogen analysis

After drying and weighing all biomass samples, they were ground and pulverized with a hammer mill in order to analyse their nitrogen content with the Dumas method. Freed by pyrolysis and subsequent combustion, nitrogen is swept by a carbon dioxide carrier into a nitrometer. The carbon dioxide is absorbed in potassium hydroxide and the volume of residual nitrogen is measured (AOAC, 1999).

Soil coverage

Related to soil evaporation a methodology was developed to accurately estimate the soil coverage over time without plant damage. At regular times from start to harvest, a camera mounted on a mobile frame took pictures of the plot underneath. Next, the pictures were subjected to an image analysis program developed in Matlab v7.6.0 R2008a (The MathWorks Inc, 2010). Basically the specific program, accounting for the prevailing conditions and crops, turns uncovered soil in the picture to black and the covered part to white. Subsequently the relative amount of white to black pixels produces the percent canopy cover.

Rooting system

In order to map the rooting system for both crops, the technique described by Vansteenkiste et al. (2014) was used. It involves a combination of imaging roots on soil trench walls and taking soil ring cores to determine root length density. During the growing season the rooting systems were laid out by taking pictures of slices of the soil profile around the plant. For cauliflower, each 2cm a plot wide 60 cm deep soil trench was dug perpendicularly to the row and repeated from 10 cm till the plant itself. A digital image of the root intersection in the vertical plane was taken with a Canon PowerShot SX110 IS before creating a new vertical plane towards the plant and extracting the roots from the trench. The same approach was adopted for leek, however with horizontal planes rather than vertical ones. Therefore, a U-shaped trench was removed around the middle row and starting at the surface horizontal planes of 3 cm deep were photographed and removed for further root extraction, which was repeated until no roots were observed visually. Meanwhile, soil sample rings were placed in the final soil profile from which roots were extracted by sieving. Digital image processing of these roots allowed the estimation of the total root length according to Kimura et al. (1999). Also, the digital images of the soil intersections were processed to obtain 3D point clouds. This way the rooting depth and relative distribution of the roots were identified.

2.3 Sampling schedule

To conclude the experimental setup and data acquisition methods an overview of the sampling procedure is given in a schedule presented in Figure 2-4 which illustrates the frequency, quantity and nature of the sampling over a cauliflower-leek rotation for each of the three consecutive years.

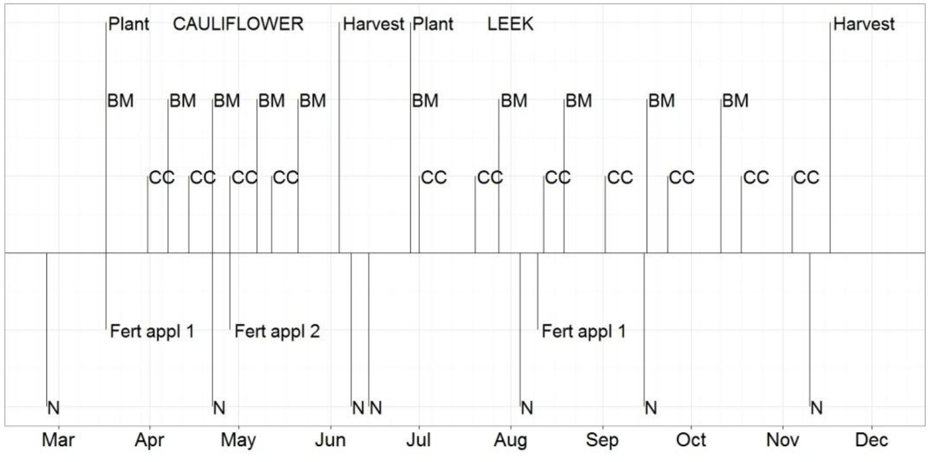

Figure 2-4 Overview of the sampling routine during a cauliflower- leek rotation regarding biomass (BM), canopy cover (CC), fertilizer application (Fert appl) and soil nitrogen (N)

Chapter 3. Default life cycle assessment

Current horticultural practices in Belgium use large amounts of inorganic fertilizers to attain high yield and quality. This practice results in an exceedance of the by law imposed residual soil nitrate threshold value of 90 kg N/ha over a depth of 90 cm at the end of the growing season (between the 1st of October and 15th of November). An experiment has been set up to monitor and evaluate the influence of four nitrogen fertilizer application rates on the growth, yield and quality of a cauliflower-leek crop rotation. Their respective impact on the environment was investigated in a life cycle assessment (LCA) considering fertilizer production and application and the auxiliary equipment and energy use. The field emissions related to fertilizer application were estimated by commonly used empirical models. This approach is referred to as the 'default' LCA and served as a reference for an alternative 'model based' LCA including more site-specific process-oriented models, that is reported in Chapter 4 (model development) and Chapter 7 (corresponding LCA output).
Nitrogen contributes to acidification and eutrophication of soil-, groundwater and surface waters, decreasing ecosystem vitality and biodiversity. Furthermore, it affects air toxicity and global change, potentially posing a threat to human health. LCA is nowadays well established as a tool for such analysis. According to the ISO 14040 (ISO, 2006), 4 steps are followed: goal & scope, life cycle inventory (LCI), life cycle impact assessment (LCIA) and life cycle interpretation.

3.1 Goal & scope

Main objective of this study was to evaluate the environmental performance of a nitrogen fertilizer application system for a yearly cauliflower- leek rotation in Flanders, Belgium. More specifically, the response to four different nitrogen doses was assessed as part of an optimisation strategy for fertilizer management.

System boundaries
The LCA was limited to a 'cradle-to-farm gate' analysis, from resource extraction till crop harvest, as the biophysical aspect of the cultivation system was of main interest considering technical sustainability (see section 1.1). Recent LCA studies for vegetable products also do identify the agricultural stage as one of the most important contributors to the environmental impact for these products (Perrin et al., 2014). Besides fertilizer production, only agricultural operations related to fertilizer application including irrigation were considered. Construction, maintenance and disposal of infrastructure and auxiliary equipment related to these operations were accounted for to the extent of data availability in the databases queried. Irrigation may directly affect water percolation with corresponding nitrate leaching and/or create more anaerobic soil conditions which favour denitrification increasing the nitrogen dioxide emissions. This is addressed by estimating the field emissions, i.c. empirically (see section 3.2) or

mechanistically (see sections 4.2 and 0). Soil preparation nor operations for planting and harvesting nor crop protection were considered due to lack of accurate information. Furthermore, these processes are independent from the applied N dose, i.e. they are similar for each treatment and thus cancel out each other by comparison. All post-harvest operations (storage, processing, transport etc.) as well as consumption (e.g. washing and cooking) and waste management of the product were excluded from the scope of the present work. Related LCA studies have shown in general that the direct environmental impact of consumption and waste handling phases were of minor importance relative to the production phase (Milà i Canals et al., 2008a; Nemecek et al., 2016; Schau and Fet, 2008). Thus, this study focused on the fertilizer application that could be managed annually to inform grower decisions and policy. The temporal boundary of each rotation system started at the planting date of cauliflower in March and ended one calendar year later, at the start of the new cauliflower season. As such, each rotation system included the inputs and emissions during, between and after the cultivation of cauliflower and leek. This is done to overcome the difficulties of attributing fertilizer application effects to just one of the crops. Indeed, nitrate leaching for instance occurs mainly during fallow periods between the crops and are thus allocated to the whole crop rotation system (Nemecek et al., 2001).

Allocation

No allocation procedure was required as crop residues were incorporated on the field and thus remained within the system. This relates to the temporal boundary of the crop rotation cycle which allocates certain impacts to separate crops.

Functional unit

The only functional flow of the system is the production of both crops. Two assessments functional units (FU) were considered: (i) one ton (t) fresh weight (FW) of both commercially harvested crops which still include part of the leaves (referred to by *COB*), and (ii) one ton FW of their respective edible part (i.e. curd for cauliflower and (white) shaft for leek, both referred to by *FRUIT*). All inputs and impacts were related to these FU’s in the LCA output. It allowed a comparison of emissions generated by the production of the same crops every year, on the same area and for different fertilizer doses. To cover the efficiency of yield on agricultural area for the different N doses, the land occupation was considered as an impact category rather than a functional unit.

3.2 Life Cycle Inventory

The life cycle inventory (LCI) consists of the compilation and quantification of relevant inputs and outputs associated with the activities within the system boundaries and related to the production of the FU, including the use of resources and emissions to air, water and soil. In this LCA study, on-farm emissions or foreground data related to specific agricultural inputs and practices were directly obtained from the experiment (e.g. fertilizer amounts and yield) and, based on them, estimated through empirical models (e.g. nitrogen emissions). Data associated with operations in the background system (e.g. fertilizer production) were taken from commonly accessed databases.

Foreground data

A detailed description is addressed in Chapter 2 and by Van Loon et al. (2011). Primary data were collected during a 3 year (2009-2011) experiment at the Experimental Station of Vegetable production at Sint-Katelijne-Waver, Belgium (Table 3-1). A cauliflower (spring)- leek (summer/autumn) rotation was treated with four different N fertilizer rates by conventional broadcast application. Calcium ammonium nitrate (CAN) was chosen as N fertilizer with the third rate (i.e. reference N dose) accordingly to the recommendation of the KNS-system (see section 2.1.1). The lowest dose was estimated aiming at minimizing nitrate leaching without significant quality loss. The actual rates were target values adjusted for the soil mineral N content. In 2011, N dose 1 was therefore even set to zero, letting the plant grow solely on residual soil nitrogen. Cauliflower received CAN in two steps, at planting and 7 weeks after, while leek only received one dose 5 weeks after planting. No phosphate based nor additional organic fertilizers were applied. Fertilizer was broadcasted by tractor and irrigation was applied when needed through a mobile sprinkler system. All auxiliary equipment inherent to the application was accounted for the lifespan and working hours allocated to the specified cultivation system.

Measurements regarding nitrogen and water were taken through plant and soil samples and retainment of leaching water. This LCA study comprised part of a completely randomized block experiment which was set up to monitor the effect of fertilizer rates on the growth, yield and quality of the crop, as well as the nitrate leaching.

The cauliflower and leek in the rotation had a growth cycle of 84 and 142 days on average and a plant density of 4 and 18 plants m^{-2} respectively. Cauliflower yielded on a yearly average 43.8, 60.5, 65.1 and 65.9 t *COB* ha^{-1} for the four N doses respectively with 17.6, 26.8, 32.2 and 30.9 t crop residue ha^{-1} which accounted for approximately 45% of the total fresh weight for all doses. The harvest comprised 23.6, 32.0, 33.4 and 32.1 t *FRUIT* ha^{-1} respectively, good for 36 to 41% of the total fresh weight. The leek cultivation returned 41.8, 43.6, 45.3 and 47.8 t *COB* ha^{-1} respectively, while the *FRUIT* consisted of 28.2, 28.5, 28.7 and 30.1 t *FRUIT* ha^{-1}, or 33, 30, 29 and 29% of total fresh weight for the four N doses respectively. Cumulatively over the rotation cycle each year, the commercial harvest was not proportionally with the fertilizer input of the different N doses. A reduction of 50% and 25% in the total amount of N fertilizer for N dose 1 and 2 respectively, decreased the harvest by only 22.5% and 6% compared to the harvest under reference N dose 3. Moreover, an increase of 25% in fertilizer input with N dose 4 only generated 3% more yield. The input-output efficiency will be accounted for in this life cycle analysis with the environmental impact associated with fertilizer production and application and the yield as functional unit.

A pairwise Tukey's studentized Range test (Figure 3-1 and Figure 3-2) was performed on the (fruit) yield of both crops for the subsequent years and different N dose rates to compare their respective means and test significant differences. The lowest N dose rate generated significant differences in total fresh yield from all other N dose rates each year. Except, the mean yield of leek shafts in 2009 was not significantly different from those of N dose 2 or 3. N dose 3 & 4 never generated significant yield differences of fresh weight or fruit, except in 2011. The same is valid regarding N dose 2 & 3, including leek yields in 2011. In general the differences in means between N dose rates were significant for leek, rather than for cauliflower.

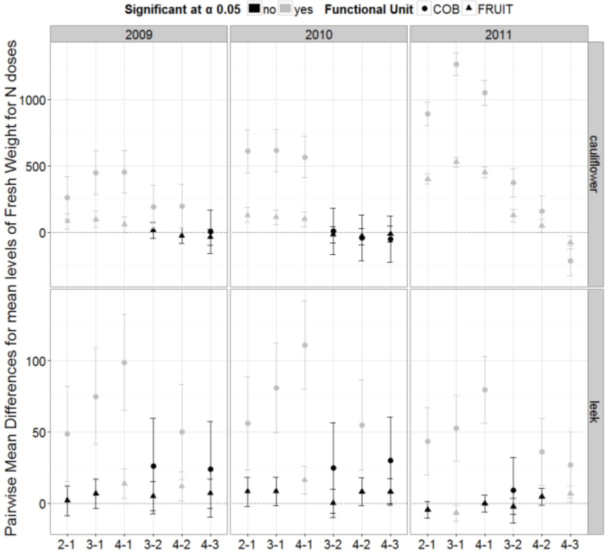

Figure 3-1 Pairwise Tukey's Studentized Range (HSD) Test for yield as *COB* and *FRUIT* for N dose rates (1-4). The N dose pairs for which the interval crosses 0, are not significant at α of 0.05.

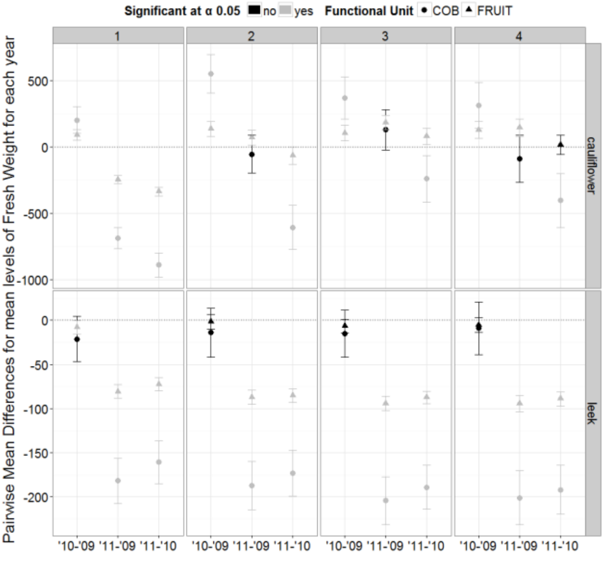

Figure 3-2 Pairwise Tukey's Studentized Range (HSD) Test for yield as *COB* and *FRUIT* for year levels. The year pairs for which the interval crosses 0, are not significant at α of 0.05

Table 3-1 Overview LCI data from a 3 year experiment on a cauliflower-leek rotation with empirically estimated field nitrogen emissions (NH_3: ammonia; N_2O: nitrous oxide; NO_x: nitric oxide and NO_3: nitrate)

	2009				2010				2011			
N dose	**Cauliflower**		**Leek**		**Cauliflower**		**Leek**		**Cauliflower**		**Leek**	
Yield [t FW ha^{-1}] *COB/FRUIT* with crop residue within brackets												
1	48.1/26.3 (+22.7)		40.9/33.6		53.3/29.0 (+20.4)		45.4/32.0		29.9/15.6 (+9.7)		39.2/19.1	
2	53.0/29.9 (+26.7)		45.5/33.9		68.8/34.4 (+31.2)		43.7/33.5		59.6/31.8 (+22.4)		41.6/18.1	
3	58.9/30.5 (+32.8)		46.4/34.9		69.3/33.5 (+34.3)		44.8/33.6		67.2/36.1 (+29.6)		44.6/17.8	
4	59.2/29.6 (+30.5)		51.1/36.1		70.0/33.1 (+34.9)		47.1/35.0		68.4/33.7 (+27.4)		45.3/19.1	
CAN fertilizer [kg N ha^{-1}] with target mineral N values in the root zone within brackets												
1	30(50) +43(100)		40(150)		24(50) +34(100)		17(100)		0(22) +0(50)		0(67)	
2	80(100) +35(150)		80(200)		74(100) +64(170)		75(175)		51(81) +53(137)		50(104)	
3	130(150) +25(200)		100(250)		124(150) +108(240)		106(250)		105(140) +75(223)		96(142)	
4	180(200) +18(250)		140(300)		174(200) +141(310)		143(325)		164(200) +133(310)		75(249)	
Irrigation [m³ ha^{-1}]												
1/2/3/4	2142				1400				1564			
Field emissions [kg N ha^{-1}] (gaseous losses of NH_3, N_2O and NO_x; leaching loss of NO_3)												
	NH_3	**N_2O**	**NO_x**	**NO_3**	**NH_3**	**N_2O**	**NO_x**	**NO_3**	**NH_3**	**N_2O**	**NO_x**	**NO_3**
1	4.1	1.9	0.2	34.1	3.4	1.5	0.2	34.1	0.8	0.5	0.1	33.3
2	6.3	2.9	0.3	34.1	7.4	3.3	0.3	34.1	5.3	2.4	0.2	33.3
3	8.8	3.8	0.4	34.1	10.9	4.8	0.5	40.0	9.0	4.0	0.4	33.3
4	10.1	4.7	0.5	48.8	13.6	6.7	0.7	107.9	11.4	5.4	0.5	76.8

Field emissions related to fertilizer application

Field emissions were defined as flows of potentially polluting substances into the environment, directly associated with fertilizer management of arable crop production on the field. Emissions of ammonia (NH_3) and nitrous and nitric oxide (N_2O and NO_x) to air and leaching of nitrate (NO_3) from the soil were assessed (see Table 3-1) through commonly applied empirical models (see Table 3-2) as mentioned in Nemecek and Schnetzer (2012) and Perrin et al. (2014). The calculation procedure was written and executed in the open source software R (R Core Team, 2016) by this work's author.

Table 3-2 LCI method to estimate nitrogen field emissions

Emission	Emission factor (EF)	Reference
NH_3	EF % of $N_{fertilizer}$ ~fertilizer type	Asman 1992
NO_3	~N_{upt}, N_{inp}, $frac_{Nleach}$, N_{miner}, soil depth	Richner 2011 (SALCA-NO_3)
N_2O	EF = 1% of ($N_{fertilizer}$+$N_{cropres}$+NH_3 loss) + 0.75% of NO_3	IPCC 2006
NO_x	EF = 21% of N_2O loss	No reference

Ammonium contained in fertilizers can easily be converted into ammonia and released to air. It contributes to acidification and eutrophication of the ecosystem. The volatilisation of NH_3 was calculated with a constant emission rate of the nitrogen fertilizer applied, provided by Asman (1992), i.c. 2% of CAN-N applied.

$$NH_3 - N = 0.02 * N_{CAN} \qquad (1)$$

where $NH_3 - N$ is the amount of ammonia emitted (kg N ha^{-1});
N_{CAN} is the amount of N applied with *CAN* as fertilizer (kgN ha^{-1}).

Nitrate is either supplied directly to the soil by fertilizers or being produced by microorganisms in the soil through nitrification of ammonium, which in turn is supplied by fertilizers as well or formed through mineralisation of soil organic matter. The main outflow is through uptake as a nutrient by the plants. In periods of heavy rainfall, however, precipitation exceeds soil evaporation and plant transpiration eventually leading to percolation to the groundwater. Once groundwater reaches the surface under soil saturation conditions, NO_3 contributes to eutrophication and also induces emissions of N_2O, a major greenhouse gas. The SALCA-NO_3 model (Richner et al., 2014) was applied to calculate the expected NO_3 leaching considering not only crop rotation, soil cultivation, nitrate fertilizing but also nitrate mineralisation from the soil organic matter, nitrate uptake by the plants and various soil conditions. The calculation is based on monthly differences between the amount of mineralized nitrate in the soil, nitrogen input by mineral fertilizers and the nitrate uptake by the plants. Furthermore, the nitrate leaching risk from fertilizer application during inappropriate time periods is taken into account. No leaching is assumed during intensive vegetation because the evapotranspiration is similar or higher than the precipitation. During this period the respective nitrogen inputs and outputs are accumulated over multiple months before the calculation of potential nitrate leaching.

$$NO_3 - N = \sum_{m'} \left[f_{ch} * f_{cr} * N_{min} + f_{risk} * f_{sd} * N_{fert} - N_{upt} \right] \tag{2}$$

where $NO_3 - N$ is the amount of N leached (kg N ha^{-1});
f_{ch} and f_{cr} are correction factors for clay and humus content (i.c. not required as clay content < 20% and humus content < 3%) and incorporation of crop residues (i.c. +43% after cauliflower harvest) respectively;
N_{min} is the amount of monthly mineralized nitrogen (kg N ha^{-1}) increased in case of intense soil cultivation in the respective month (see Table 3-3);
f_{risk} and f_{sd} are correction factors for risk of nitrogen leaching due to fertilizer application (as a function of crop and month) and the useful soil depth (if less than 100cm) respectively on N_{fert}, the amount of monthly applied N fertilizer (kg N ha^{-1});
N_{upt} is the amount of N taken up monthly by the crop (kg N ha^{-1}) generated by proportionally dividing the harvested N for each dose according with the data provided by Feller et al. (2011) (see Table 3-4).

Table 3-3 Expected nitrogen mineralisation (N_{min} , kg N ha^{-1}) per (aggregated) month(s) without (*ext.*) or with (*int.*) intensive cultivation according to Richner et al. (2014) applied to a cauliflower- leek rotation

	1	**2**	**3-4-5**	**6**	**7-8-9-10**	**11**	**12**	**Tot**
$\boldsymbol{ext.N_{min}}$	0	0	6+9+12	15	17+21+23+12	6	0	121
$\boldsymbol{int.N_{min}}$	0	0	10+15+20	25	29+38+38+20	10	0	205

Table 3-4 Expected nitrogen uptake (kg N ha^{-1}) of cauliflower (Cauli) and leek as a function of the week after planting according to Feller et al. (2011)

	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**	**13**	**14**	**15**	**16**	**Tot**
Cauli	1	1	3	7	18	39	64	65	38	15	-	-	-	-	-	-	251
Leek	1	2	3	4	7	9	13	20	28	35	37	33	23	14	8	3	240

This led to nitrate leaching (see Figure 3-3) that is assumed to occur, besides at the initial phase of cauliflower cultivation in March depending of the year and N dose, mostly in June which includes the fallow period between cauliflower harvest and the transplanting of leek. Also in November after the leek is being harvested, a certain amount leached in each year and for each N dose application rate.

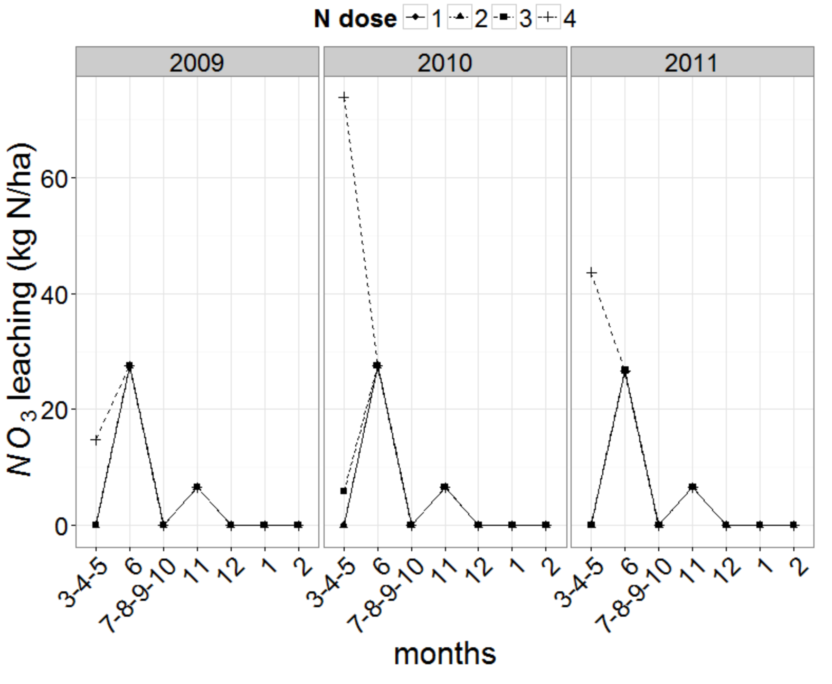

Figure 3-3 Expected nitrate (NO_3) leaching for each N dose scenario for three consecutive years, calculated by the SALCA-NO_3 method. The first two months belong to the temporary boundary of the year before in which the crop rotation started.

Nitrous oxide (N_2O) is produced as a by-product during nitrification but mainly as an intermediate product in the denitrification process. It contributes to the total greenhouse gas emissions with a high impact (298 kg CO_2-eq. per kg N_2O). Direct and induced emissions of N_2O are estimated by the IPCC method Tier 1 (IPCC, 2006). Direct emissions originate due to fertilizer application and crop residue incorporation, while induced emissions occur after volatilisation of ammonia and after nitrate losses from surface water.

$$N_2O - N = 0.01 * \left(N_{fert} + N_{cr}\right) + 0.01 * NH_3 - N + 0.0075 * NO_3 - N \qquad (3)$$

where $N_2O - N$ is the amount of N emitted as N_2O (kg N ha^{-1});
N_{fert} and N_{cr} are the amounts of N applied through fertilizers and crop residue respectively;
$NH_3 - N$ and $NO_3 - N$ are the amounts of N lossed through ammonia volatilisation and nitrate leaching respectively (kg N ha^{-1}).

And finally, nitrogen oxide (NO_x) is as well produced during (de)nitrification processes, contributing to human toxicity, acidification and eutrophication. Emissions of NO_x from fertilizers and the soil were considered as 21% of the N_2O loss (Nemecek and Schnetzer, 2011).

$$NO_x - N = 0.21 * N_2O - N \quad (4)$$

where $NO_x - N$ and $N_2O - N$ are the amounts of N emitted as NO_x and N_2O respectively (kg N ha^{-1}).

Background data

The LCA accounts for the emissions and processes related to fertilizer production and their application like fuel use and infrastructure. These general data as well as the characterisation factors, translating input data and field emissions into the environmental impact, were acquired from the life cycle inventory database Ecoinvent v2.2 corresponding with the LCIA methods mentioned beneath (Frischknecht et al., 2005).

3.3 Life Cycle Impact Assessment

The impact assessment (LCIA) procedure was developed by Carlos Bojacá (Bojacá et al., 2014) and Reindert Heuts (this work and cf. ‘List of publications’ section). It is written and executed with the open source R software (R Core Team, 2016) according to midpoint CML 2001 method (Guinée et al., 2002) and the Cumulative Energy Demand (CED, (VDI, 1997)) which resulted in a selection of 6 impact categories as presented in Table 3-5. The area occupation was thereby added as the inverse of the yield, representing an area efficiency indicator. The emissions to the environment from all industrial and agricultural subprocesses related to the fertilizer management are classified and characterized into the impact categories with corresponding unit equivalents.

Table 3-5 Overview of selected impact categories and their unit equivalents

Impact category	Acronym	Unit
Acidification potential	AP	kg SO_2 (sulphur dioxide)-eq.
Global warming potential	GWP	kg CO_2 (carbon dioxide)-eq.
Eutrophication potential	EP	kg PO_4 (phosphate)-eq.
Human toxicity	HT	kg 1,4-DCB (dichlorobenzene)-eq.
Cumulative energy demand	CED	MJ-eq.
Land occupation	LO	ha

An overview of the environmental profiles of each N dose scenario, related to the two functional units kg *COB* and kg *FRUIT*, and for three consecutive years is presented in Figure 3-4. It shows for each impact category the impact relative to the one of N dose 3, which was considered as the default management advised by KNS (Lorenz et al., 1985). Furthermore, in Figure 3-5, relatively for each N dose scenario, the contribution of three system components to each impact category is shown (similar for both functional units): *Fertilizer use*, reflecting the field emissions, *Fertilizer production* and *Auxiliary* including the equipment and energy use for the fertilizer application.

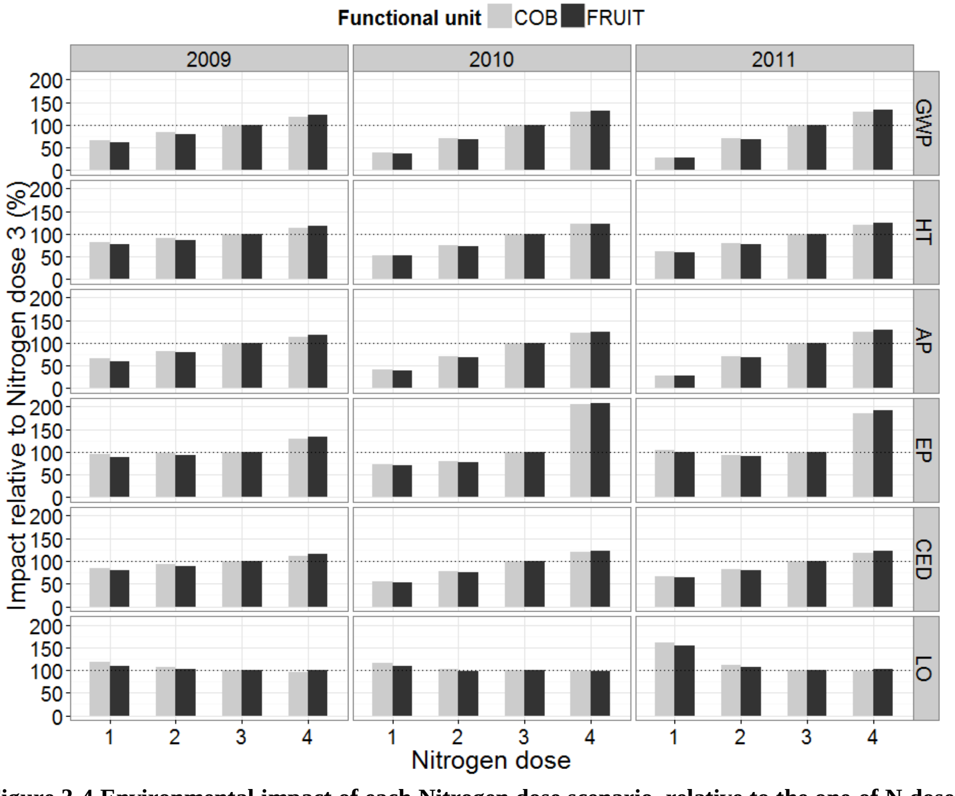

Figure 3-4 Environmental impact of each Nitrogen dose scenario, relative to the one of N dose 3 (i.e. recommended by KNS). The 6 impact categories are shown, related to the respective functional units *COB* and *FRUIT*, and for 3 consecutive years (GWP= global warming potential, HT= human toxicity, AP= acidification potential, EP= eutrophication potential, CED= cumulative energy demand and LO= land occupation).

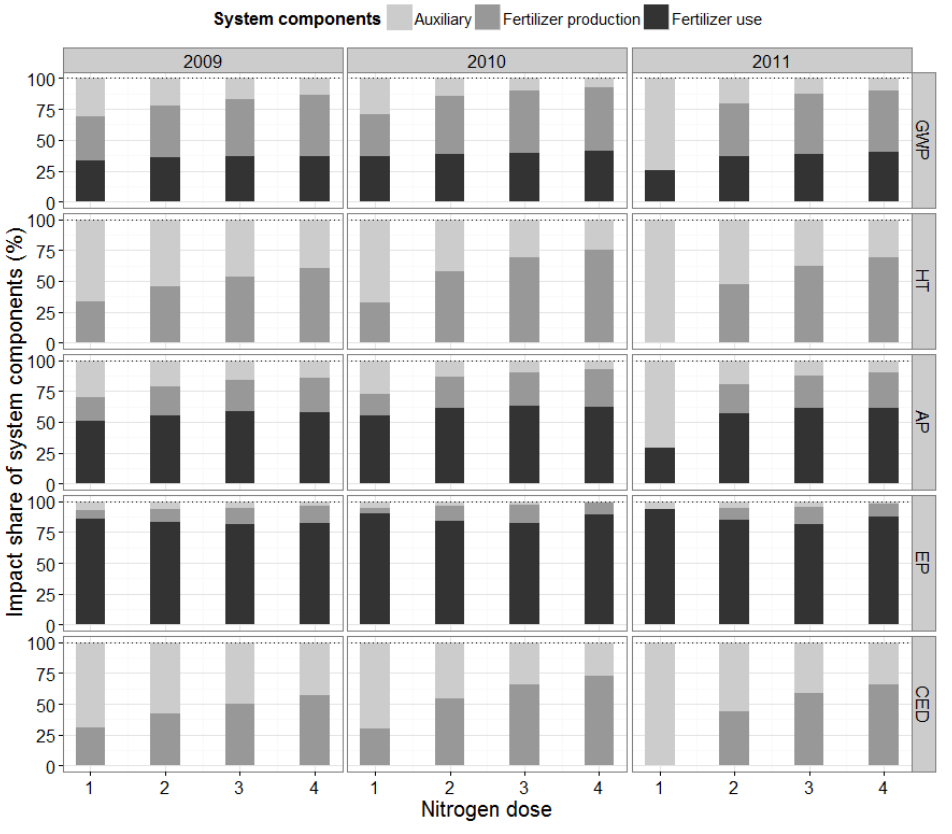

Figure 3-5 The relative contribution of the 3 considered system components (fertilizer production, fertilizer use and auxiliary components) to the respective impact categories (GWP= global warming potential, HT= human toxicity, AP= acidification potential, EP= eutrophication potential and CED= cumulative energy demand) for each N dose scenario and for 3 consecutive years (results per kg *COB* and per kg *FRUIT* are similar).

3.4 Life Cycle Interpretation

Interpreting LCIA results and gaining insight in the overall environmental performance of a system is not straightforward. It depends on the relative importance of each impact category and the trade-off between yield and costs, including potential environmental costs. Overall, the scenarios with the lower doses 1 and 2 show a lower environmental impact compared to the burden with N dose 3, while the higher N dose 4 scenario generates a higher impact. Only for the land occupation the opposite is valid, although the differences are less distinct, except for N dose 1. With the *FRUIT* yield as functional unit, the respective decrease and increase in impact compared to the reference scenario is slightly more pronounced.

Global warming (GWP) and acidification potential (AP)

The scenarios show a similar trend for GWP and AP. Over the three years the lower N doses 1 and 2 have an impact of 30-65% and 70-82% respectively compared to that of N dose 3 related to the commercial yield *COB*. N dose 4 increases the GWP and AP of N dose 3 by 15-29%. Per kg *FRUIT* the impact is an additional 1-5% off, i.e. lower for N dose 1 and 2 and higher for N dose 4 compared to the reference.

The biggest contributors to these impact categories are the fertilizer production and their induced field emissions. Due to the fertilizer use 30-41% of the GWP are the N_2O emissions which have a CO_2-equivalent of 298 kg. These are mainly fertilizer related and indirectly from NO_3 leaching according to the empirical calculation (see equation (3)). For AP, the share is even 51-62% (except for the 30% in the case of N dose 1 for 2011) due to ammonia volatilisation (and NO_x to a lower extent) from fertilizer application.

Human toxicity (HT) and cumulative energy demand (CED)

Also for HT and CED, the environmental impact is similar. The toxic emissions and energy demand are both 15-45% and 9-24% lower for N dose 1 and 2 respectively compared to N dose 3 over the three years. N dose 4 shows a 12-21% increase for both categories. The scenarios comprise an extra 2-6% difference to N dose 3 per kg *FRUIT*.

The share of fertilizer use is negligible for HT to non-existing for CED compared to the production of fertilizers and auxiliary equipment including energy use.

Eutrophication potential (EP)

For all N dose scenarios, 81-93% of the EP is caused by field emissions related to fertilizer application, mainly due to nitrate leaching. Based on equation (2), leaching is in essence calculated as the balance of fertilisation (+) and nitrogen uptake (-) as the mineralisation per month is equal each year for each N dose. For the lower doses 1 and 2, the commercial yield (*COB*) is relatively high enough to decrease the EP with 4-26% and 3-20% respectively compared to the reference, with exception of N dose 1 in 2011. The EP for N dose 4 on the other hand, is 28-

106% higher as the yield does not compensate the N fertilizer input. Also within this impact category, the differences with the N dose 3 scenario are an additional 2-7% lower and higher per kg FRUIT for the respectively lower and higher N dose scenarios.

Land occupation (LO)

The inverse of commercial yield (*COB*) efficiency results in a land occupation or occupation that is about 17% (62% in 2011) and 1-10% higher for respectively N dose 1 and 2 compared to the LO of N dose 3. The scenario of N dose 4 requires 2-4% less area. Except for N dose 1 which still needs 10% (55% in 2011) more area, the LO per kg *FRUIT* is not necessary inversely proportional with the N dose. The LO of N dose 2 and 4 differ by 1 to 8% lower or higher than that of N dose 3 depending on the year.

3.5 Discussion and conclusion

The LCA assessed and compared the environmental impact of the nitrogen fertilizer application in a cauliflower-leek rotation under different N doses. The assessment showed that increased fertilizer application does not result in a sufficient increase in yield to justify additional emissions and be environmentally favourable.

3.5.1 Yield versus area

Although the productivity and land occupation favour the higher N dose, it is not necessarily true in terms of kg *FRUIT*. Considering the edible part of the crop, the yield efficiency for N dose 2 in 2010 and N dose 4 in 2011 were respectively higher and lower than for N dose 3. Given the food waste problem in industrialized nations (Gruber et al., 2016), the environment could benefit from future assessments taken into account this ‘true’ productivity. On the other hand, a shift on the demand side towards rational consumption could stimulate more sustainable production as the size of each crop does not have to be as perfect and as big as possible. If the yield under reference N dose 3 is still required, the same target could be reached under a lower N dose, but on a larger area. Based on an average approximation of the results of this study, excluding the lowest fertilizer scenario in 2011 for which the N dose was reduced to zero, 25% more area under N dose 1 with 60% of the fertilizer input would equal the productivity under N dose 3, even with 10% more leek, while the impact regarding global warming, acidification, human toxicity and energy demand would remain 10 to 20% lower. Only the eutrophication potential would be similar between both scenarios. A more accurate assessment however is required to account for the impact related to compensate the potential change of land use on the additional required area.

3.5.2 Effect of impact reduction strategies

Application of a lower N dose would benefit the environment, but entails a lower commercial yield. As long as the production costs per unit yield is the only factor for a grower, his management will not change because of environmental implications. Potential internalisation of environmental externalities might alter his policy. Additional costs for (in)direct threats to human and ecosystems e.g. potential water pollution or greenhouse gas emissions would imply an intensive monetisation. Emission costs could be derived from mechanisms like the EU emissions trading system for addressing climate change (EU ETS; European Commission, 2015) or the cost for remediation. Increased groundwater treatment would bring extra operational costs, but at the same time generate even more greenhouse gas emissions. This 'pollution swapping' should be accounted for or , ideally, avoided (Bouraoui et al., 2011).

Within a sustainability context, a proactive approach might be more appropriate. Based on the LCA results and assuming the share of renewable energy sources will increase over time, efforts should be made to reduce emissions of nitrogen pollutants. They are a major source for climate change, acidification and eutrophication as also assessed by former studies (Cederberg, 2010; Milà i Canals et al., 2008b; Nemecek and Erzinger, 2005; Williams et al., 2006). When it comes down to support decision making towards a more environmentally favourable management based on the LCA approach and the results as presented, potential mitigation strategies should involve less mineral fertilizers and avoid crop residue incorporation.

Less mineral fertilizer

Field emissions of ammonia, nitrate, and nitrogen oxide are directly related to the amount of N applied. Less mineral fertilizers could be compensated by a larger area as mentioned above or potentially by an organic alternative. In the assessment, application of manure and/or compost does avoid the production and use of synthetic fertilizers and the corresponding impact, but it entails different processes and their impact consequently. The burdens of the organic fertilizer can be debited to the animal production or composting system, except for its spreading and subsequent nitrogen losses. Given the substitution of mineral fertilizer by the threshold in Flanders, Belgium of maximum 170 kg N from animal manure (VLM, 2017) and the empirical estimation addressed in Nemecek and Schnetzer (2012), the ammonium emissions could be increased by two till tenfold depending of the type of manure and application method. The acidification potential however could be limited to status quo until a fivefold increase considering the avoided burden from synthetic fertilizer production. Regarding nitrogen oxide, the emissions according to the IPCC guidelines (IPCC, 2006), are independent of the source of N fertilizer, but are induced by a change in ammonia and nitrate leaching. The benefit of the organic fertilizer alternative would be the avoided global warming potential and human toxicity from the synthetic fertilizer production in the order of 1000 kg CO_2 and 350 kg 1,4-DCB-equivalents respectively, which would outweigh the induced N_2O and NO_x emissions from ammonia and nitrate leaching with a maximum of 300 kg CO_2- and 1 kg 1,4-DCB- equivalents respectively. Following the estimation procedure of Richner et al. (2014) the use of 110 kg N ha^{-1} from manure would increase the mineralisation up to 10% (and the next year between 5.5 and 11 kg) which would increase the nitrate leaching and thus eutrophication potential accordingly. Then again, the application of a different kind of fertilizer would require an additional application of broadcasting which requires more energy. The cumulative energy demand approaching 380 MJ ha^{-1} however is only a factor 30 of the avoided energy use of producing the synthetic fertilizer. Similar for compost, although not clearly addressed and with a lower 'working coefficient' releasing nitrogen slower over time, a comprehensive comparison of different fertilizer management scenarios in an LCA context is more complex and requires a critic review of the presented methodology. Research into the effects of N fertilisation on N_2O fluxes has yielded somewhat contradictory results. Whether or not the emissions would be reduced, depends mainly on water management and soil conditions besides the type of fertilizer (Aguilera et al., 2013).

Avoid crop residue incorporation

To prevent more leaching, an (additional) option could be to carry off the crop residue towards a composting facility and assess the impact. Given the removal of 32.8 ton fresh weight or 90 kg N ha^{-1}, it would decrease the nitrate leaching and eutrophication potential by 10% and the global warming in the order of 30%. On the other hand, a by-product is generated that has to be processed and requires an extension of the system boundaries. Composting mainly entails organic material decay and energy use. Depending on the technology type, in the order of 1400 to 13500 kg CO_2 equivalents would be emitted, although around 95% is of biogenic nature taken up during plant growth (Boldrin et al., 2009). As the latter is not accounted for in the assessment, the composting scenario could be a saving or net load for the environment compared to that with soil incorporation, let aside the potential yield loss that could be generated by removing a nitrogen source.

3.5.3 Limitations of the standard empirical approach

Caution is advised interpreting and pass on the LCA outcome as assessed. Although transparency issues arose, more and more studies within an LCA context apply indeed empirical estimations to quantify field emissions due to fertilizer use. They refer to the general guidelines (Audsley et al., 1997; Nemecek and Kägi, 2007) or the nitrogen balance of Brentrup et al. (2000) in order to reduce the complexity requiring minimal data input and being easy to perform. Downside of this approach is the overlooking of the local soil, climatic and agricultural management factors considering their diversity and variation in time that affect the carbon-nitrogen dynamics and the related effect on the environmental impact (Bessou et al., 2013a; Giltrap et al., 2010; Peter et al., 2016).

Synthetic fertilizers were introduced to overcome the lack of control of nitrogen release from organic sources to meet the N demand of the crop at the right moment. Yet, the application in practice is still limited to the early cultivation stage and poor weather and/or soil conditions could nullify the advantage of mineral fertilizers considering their volatility. Given the simplistic and aggregated estimation of field N emissions, the effect of fractionated fertilizer application for instance would be assumed non-existent. Thus, potential benefits of mitigation strategies might not be fully addressed, nor through the simplistic field emission estimations, nor through the impact categories, let aside be recognized as policy drivers (Aguilera et al., 2013; Martínez-Blanco et al., 2011; Peter et al., 2016). Long term advantages as soil fertility and workability or soil water holding capacity are hardly quantified.

As natural variability is inherent in agricultural production, future climate and soil conditions could alter the whole N flow through the crop-soil-air environment and shift the most favourable fertilizer management. No effect of precipitation (only indirectly accounted for in the monthly default mineralisation values) nor soil water conditions are considered although they play an important role (Peter et al., 2016).

Between the two crop cultivations in June and after leek harvest in November, only mineralisation occurs which is not compensated by N uptake of the crop and thus generates a peak in nitrate leaching. The expected leaching during fallow periods in winter is not reflected by the results, which could already be anticipated from the estimation procedure given the lack of mineralisation and fertilizer application in fallow winter months. The amount of 6.6 kg N ha^{-1} in November is far from the threshold of 90 kg N ha^{-1} which is exceeded frequently at open field vegetable production in Flanders as mentioned in the introductory chapter. Given the monthly time step and the interpretation of ‘intensive’ cultivation and N uptake of only small leek plantlets at the end of June, the first peak of nitrate leaching might be a methodological artefact of the calculation procedure by Richner et al. (2014) or at least out of proportion with the rest of the year. Measurements of the soil N samples from the experiment did not show agreement with this estimation. Furthermore, the effect in June is enhanced because of cauliflower residue incorporation that increases the mineralisation.

Ultimately, the effect of potential mitigation strategies, i.e. relatively more organic fertilizers, crop residue removal or others like cultivation timing and/or multiple split fertilizer application through fertigation should be assessed more accurately in order to support decision making. Especially the interaction between climate, soil conditions and crop growth and the induced implications from mitigation strategies on the whole system being assessed, requires more insight. A dynamic evaluation would be advised in order to quantify the environmental impact of the nitrogen fertilizer application management in a crop rotation system and to suggest more sustainable alternatives.

Chapter 4. The integrated crop-soil model

To evaluate and improve agricultural systems, an integrated model is developed that represents the dynamic crop-soil processes in a systems context. The full integrated model compilation and implementation in open source R software was carried out by this works' author. The series of process based submodels, linked into a system model, have in general a mechanistic structure. Yet, empirical information and submodels are inevitable incorporated from literature or through pedo-transfer functions with data from the measurements. This work focused on the dynamic and process based characteristics of the model, rather than justifying the model 'type' for which the line of classification is not always clear (Wallach et al., 2014). Aiming at a generic and extendable model, the R-code was developed in a modular way as all major processes were written as parameterized R-functions. This makes adaptations to other crops, soil and climate conditions very straightforward, as well as incorporation of alternative submodels.

As addressed in the following description of each submodel, the current development was based on existing models, widely applied and tested, yet implementing recent adaptations to improve accuracy, while maintaining a balance between model genericity and complexity. The model is expected to facilitate the strategic decision making and operational recommendations as a function of environmental and management conditions.

Driven by daily meteorological data (precipitation, solar radiation, air temperature,...), soil properties (bulk density, field capacity,...) and agricultural management (irrigation, fertilizer application,...), the crop-soil model simulates at field scale the soil temperature, crop growth, water transport and soil organic carbon and nitrogen dynamics. It thereby predicts the emissions of environmental pollutants to the air (carbon dioxide, ammonia, nitrous and nitric oxide) and to the ground water (nitrate).

The model runs on a daily time step, with exception of the crop growth module in which the photosynthetic mechanism is estimated based on hourly data and CO_2-assimilation is aggregated up to a daily increment of plant biomass. As presented in Figure 4-1, 10 modules are sequentially implemented by the main program, all of them being described in the following sections. If crop stress might be expected, i.e. the supply of water and/or nitrogen does not meet the demand from the crop, a soil deficiency factor (*SDF*) from the uptake submodels will be implemented in the crop growth submodel. This will limit the potential growth in accordance with the supply that is available. This implies that the submodels of crop growth, evapotranspiration and, rather for control, uptake are rerun before the last submodels for evaporation and diffusivity end the daily loop (Figure 4-1).

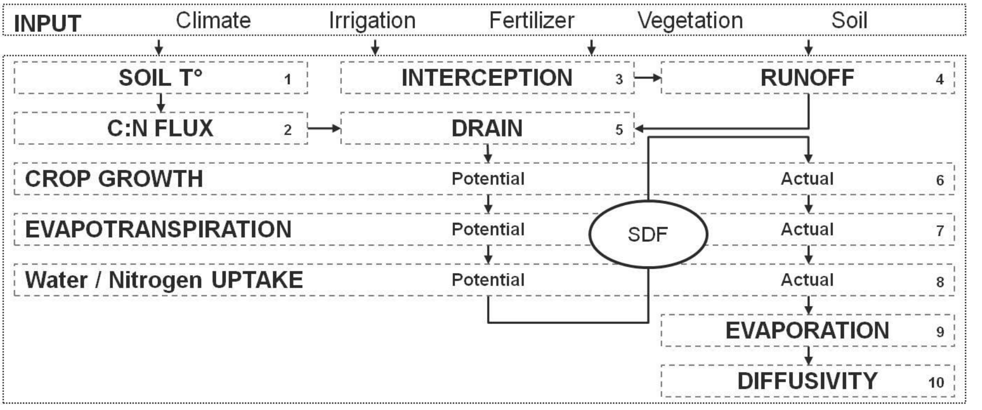

Figure 4-1 Overview model structure

4.0 Main program

In the main module the input requirements regarding simulation control, climate, soil properties and crop management are defined and assigned to the submodules. This input is considered to be fixed and not subjected to calibration or sensitivity analysis. Next, the flow of the whole model is set and the output is compiled.

General data required in one or more modules are listed below:

1. Simulation control settings:
    - Reference date (*RefDate*, sets the Julianday), start date of simulation (*NSTART*), length of simulation (*NDAYS*).
    - Geographical settings: altitude (meter above sea level), latitude (degrees, positive for northern hemisphere, negative for southern) and longitude (positive degrees, west of Greenwich, England).
2. Climate:
    - Hourly data of solar radiation (W m^{-2}), air temperature (°C), relative humidity (%), precipitation (cm) and wind speed (m s^{-1}) are required by the crop module and aggregated to daily values for other modules.
3. Soil properties:
    - Layer thickness (*LT*, *cm*): it is recommended to limit upper, intermediate and deeper layers to respective 10, 20 and 30cm thickness, e.g. *LT* needs to be sufficiently small to accommodate the functional simulation procedures needed to reasonably predict plant water status (Ritchie, 1998).
    - Soil properties: soil bulk density (*BD*, g cm^{-3}); soil water content (cm^3 cm^{-3}) at lower limit (*LL*), at field capacity (*FC*) and at saturation (*SAT*); pH, organic carbon content (*OC*, %), cation exchange capacity (*CEC*, $cmol_c$ kg^{-1}) and texture (clay, loam and sand, %) per soil layer.

- Initial contents of soil water ($cm^3\ cm^{-3}$) and mineral nitrogen (ammonium and nitrate, $g\ cm^{-3}$) per soil layer at start date of simulation, with the latter being constrained so that a minimum amount (*AmMin* and *NiMin* respectively (mg N / kg)) remains in the soil layers.

4. Crop management:
   - Planting dates for each cultivation (for calibration procedure the harvest dates were also provided, including the date of curd initiation during cauliflower cultivation).
   - Plant density (plants m^{-2}).
   - Seedling initial properties comprising (i) the dry matter of the different plant organs (leaf, stem and curd; the root dry matter (g $plant^{-1}$) is estimated as a function of the above ground shoot biomass although measurements could be used as well), and (ii) the initial Specific Leaf Area (SLA, $cm^2\ g^{-1}$).
   - Virtual root distribution: a relative root density distribution distributes daily added root dry matter over the current rooting depth.
   - The crop developmental stage (*DVS*) is estimated at the start of the simulation (detailed explanation under crop module 0).
   - Irrigation: daily amounts of water (cm).
   - Fertilizer application of organic crop residues and/or manure, and inorganic fertilizers and/or urea: day and depth (cm) of application, amount (kg C(organic) or N(inorganic) ha^{-1}) and in case of organic input the C:N ratio (-).
5. Preset of 2 output files: a set of variables calculated per soil layer and a set of variables also calculated daily, but independent of the layer structure.

Depending of the module, transformations between relative concentrations and absolute amounts might be required with following factors in bold:

$$[mg\ kg^{-1}] = \frac{\mathbf{10}}{\boldsymbol{LT} * \boldsymbol{BD}} * [kg\ ha^{-1}]$$

$$[kg\ ha^{-1}] = \boldsymbol{LT} * \mathbf{100000} * [g\ cm^{-3}]$$

$$[cm] = \boldsymbol{LT} * [cm^3\ cm^{-3}] \quad \text{(for soil water)}$$

4.1 SoilTemp submodel

Soil temperature is an important component as it affects crop growth and development, carbon and nutrient cycling, water dynamics and the intensity of physical, chemical and microbiological processes in the soil. Based on the module in CERES (Jones and Kiniry, 1986) and EPIC (Williams et al., 1983) the soil temperature follows a cosine function of Julian day with an exponentially decreasing amplitude with depth, and is modified by a five-day moving average of the soil surface temperature. Each day i and for each soil layer depth z (cm, taken zero at the surface) the average soil temperature T_s^i is calculated by,

$$T_s^i(z) = T_a + \left(\frac{T_{amp}}{2} * \cos\left(\frac{2\pi}{365} * (i - H) - \frac{z}{DD}\right) + DT^i\right) * e^{-z/DD} \tag{5}$$

where T_a and T_{amp} are respectively the mean annual air temperature and the annual amplitude of mean monthly air temperature (°C);
H is the hottest day of the year (Julian day);
DD is the damping depth (cm);
DT is the change in soil surface temperature due to actual weather conditions (°C).

Equation (5) is the analytical solution of the 1-dimensional heat flow equation for an infinitely deep and homogeneous soil and a seasonal temperature fluctuation of the soil surface temperature according to a sine wave with a period of 365 days (Jury and Horton, 2004). The cosine term allows subsurface temperature changes to lag behind those of the surface, thereby reaching a maximum value of (T_a+$T_{amp}/2$) for the normal surface soil temperature at the hottest day (i=H). The exponential function of the ratio of the layer depth z and damping depth DD represents the difference in temperature between surface and subsurface layers. DD is the depth in the soil at which variation in temperature due to changes in climatic conditions is limited to a fraction $T_{amp}*e^{-1}$ of T_a. It depends upon average soil bulk density and water content as follows:

$$DD = DD_{max} * e^{\ln\left(\frac{500}{DD_{max}}\right)*\left(\frac{1-\S}{1+\S}\right)^2} \tag{6}$$

$$DD_{max} = 100 + 250 * \frac{BD_{avg}}{BD_{avg} + 686 * e^{-5.63*BD_{avg}}} \tag{7}$$

$$\S = \frac{SW}{\left(0.356 - 0.144 * BD_{avg}\right) * z_{tot}} \tag{8}$$

where *DD* is the damping depth (cm);
DD_{max} is the maximum damping depth (cm);
BD_{avg} is the average soil bulk density over the soil profile (g cm^{-3});
§ is the scaling factor for soil water (-);
SW is the total amount of soil water in the soil profile above lower limit (cm).

To account for the effect of the actual weather conditions on a particular day, the normal soil temperature course is corrected by the term DT^i as described as follows:

$$DT^i = T_{s,a}^i - \left(T_a + \frac{T_{amp}}{2} * \cos\left(\frac{2\pi}{365} * (i - I)\right)\right) \quad (9)$$

$$T_{s,a}^i = \frac{\sum_{j=i-4}^{i}(1 - alb) * (T_m^j + \left(T_{max}^j - T_m^j\right) * \sqrt{0.03 * S_{rad}^j}) + alb * T_{s,a}^{j-1}}{5} \quad (10)$$

where $T_{s,a}^i$ is the five-day moving average of the actual surface soil temperature (°C) on day *i*;
alb is the albedo of the surface (-);
T_m^j and T_{max}^j are the daily mean and maximum air temperature (°C);
S_{rad}^j is the daily global radiation (MJ m^{-2} d^{-2}).

A change in soil surface temperature with time (*DT*) is the difference in a five-day moving average of the actual surface soil temperature and the normal surface soil temperature as calculated by equation (5) with z=0 and neglecting *DT* (Jones and Kiniry, 1986; Sharpley and Williams, 1990).

4.2 C:N flux submodel

Soil organic matter (SOM) stores three to four times the amount of carbon (C) found in all living vegetation. Among the macronutrients it contains, nitrogen (N) plays a major role since it is essential for life although most of it is present in the form of organic compounds. Therefore in many ecosystems the C:N cycle controls overall soil turnover and functioning (Batlle-Aguilar et al., 2011). It is furthermore a vital model component in order to predict accurately for instance the effects of changes in climate and management on the environment, and mainly on greenhouse gas (GHG) emissions (Cannavo et al., 2008). Fixation or release of these biogeochemical elements in the soil is fundamental as a major indicator of soil fertility and for other processes which affect productivity and may burden the environment. This submodule (Figure 4-2) simulates the dynamics of both carbon and nitrogen in the soil including decomposition, with parallel mineralisation, ammonium adsorption, urea hydrolysis if applied, ammonia volatilisation and (de)nitrification. Nitrate leaching is addressed in the drain submodule (section 0) that describes the transport of water and solute. Nitrogen supply through atmospheric deposition is currently not integrated as its effect is assumed relative small considering the intensive use of fertilizers in horticultural production and it is rarely modelled (Cannavo et al., 2008).

The complex interaction of the considered N processes is represented as a system of ordinary differential equations (solved in R by the *lsoda* function) of first order that generalizes the structure of most compartment based N cycle models. Only ammonium adsorption is assessed by an equilibrium each day after the other processes within the module occurred. Each soil layer is virtually represented by soil organic matter and mineral nitrogen characterized by their respective compartments or pools with homogeneous properties. Furthermore, as field measurements show that soil profiles are rarely completely depleted of mineral N, a minimum content of each mineral N pool is set, below which mineral N is unavailable to any process (Bradbury et al., 1993a; Jones et al., 2003; Smith et al., 2010). If fertilizer is applied, depending on the type of fertilizer, the mineral N or plant material pools are immediately updated that day in the top or in multiple soil layers. Synthetic fertilizer applied by broadcasting adds mineral N to the mineral N pools of the top soil layer, while incorporation of organic fertilizers will add carbon and nitrogen to the plant material pools of all the soil layers that is reached by the incorporation depth.

All values are expressed in C or N equivalents in kg ha^{-1} and calculated for each soil layer with a daily time step.

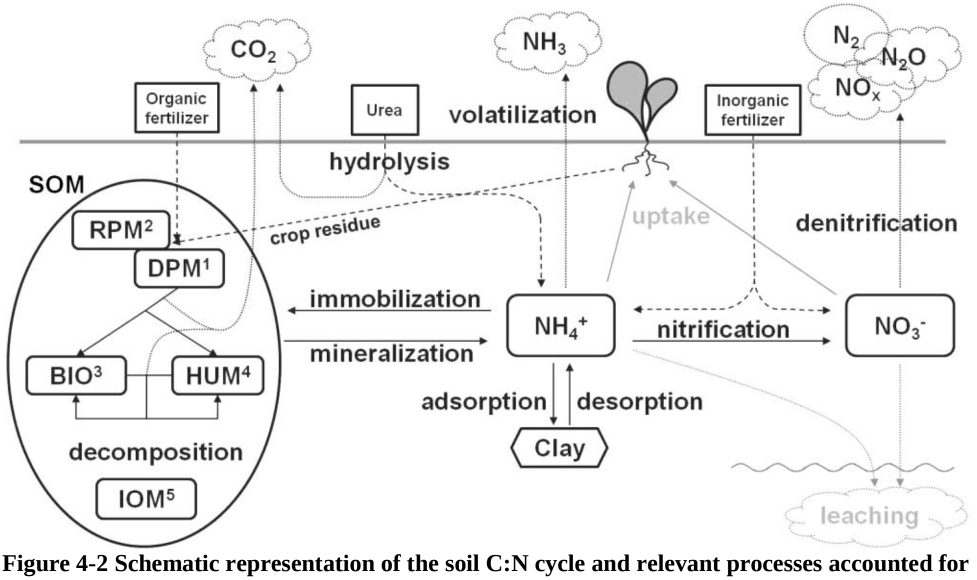

Figure 4-2 Schematic representation of the soil C:N cycle and relevant processes accounted for in the C:N flux submodel: the rounded squares represent the soil state variables, i.e. the soil organic matter (SOM, see also Figure 4-3) content, divided into 5 pools: 1) decomposable plant material (DPM), 2) resistant plant material (RPM), 3) biological pool (BIO), 4) humus pool (HUM) and 5) inert organic matter (IOM); next are the inorganic ammonium (NH_4) and

nitrate (NO_3) pool. Along with the respective processes, gaseous losses (clouds) occur: carbon dioxide (CO_2) due to SOM decay, ammonia (NH_3) due to volatilisation, nitrous (N_2O) and nitric (NO_x) oxides due to (de)nitrification; dinitrogen (N_2; circle) is emitted as well as harmless end product of denitrification. Processes of N uptake and leaching (grey) are not accounted for in this submodel, but addressed in the submodels of uptake (section 4.8.2) and drain (section 0) respectively.

4.2.1 Decomposition – mineralisation/immobilisation

The turnover of C and N in the soil organic matter (SOM) was developed based on concepts originally derived from RothC (Coleman and Jenkinson, 1999; Jenkinson et al., 1987) and SUNDIAL (Bradbury et al., 1993a), and adapted in ECOSSE (Smith et al., 2010). The structure of the model is set out in Figure 4-3. The SOM is described as pools of decomposable plant material (DPM), resistant plant material (RPM), microbial biomass (BIO), humus (HUM) and inert organic matter (IOM), each decomposing with a specific rate constant. They are also being addressed within the equations (12) - (17) by the letters *i* and *j (=1 to 5 respectively).*

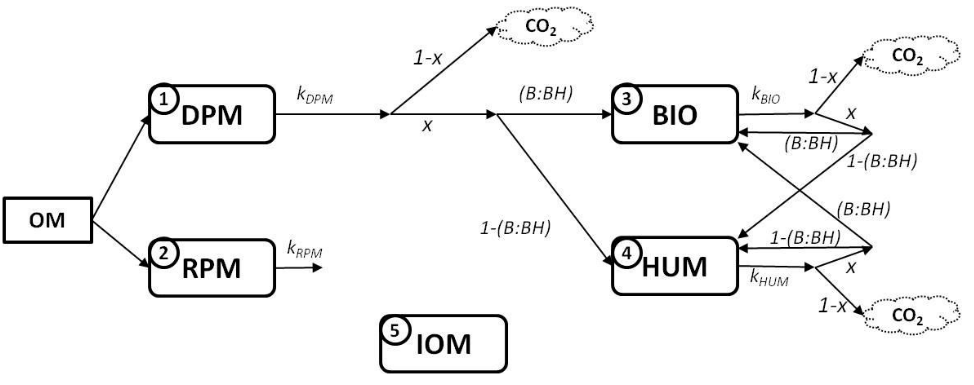

Figure 4-3 Structure of the SOM decomposition/mineralisation model: Incoming organic material (OM) is split between the decomposable (DPM) and resistant (RPM) plant material compartment. Both DPM and RPM decompose with a rate constant k_{DPM} and k_{rpm} respectively per day to form CO_2, microbial biomass (BIO) and humus (HUM). The proportion that goes to CO_2 and to BIO +HUM is determined by the clay content with x=1/(crat+1) (see Equation 15). The BIO+HUM is split with a fixed proportion of B:BH to BIO and 1-(B:BH) to HUM. Both BIO and HUM decompose to form more CO_2, BIO and HUM. A small amount of inert organic matter (IOM) is resistant to decomposition. The C:N ratios of the BIO and HUM pools determine the amount of N that is mineralised or immobilised respectively to or from the free ammonium (not shown) along with the decomposition.

Initialisation of the SOM pools can be assessed through multiple ways like an equilibrium run of the model as described in Coleman et al. (1999) or an iterative procedure as in Smith et al. (2010). Here, the initialisation of the model is based on the assumption that the SOC is at steady state under the current land use at the start of the simulation. First, an estimate for the amount of IOM-C is given by Falloon et al. (1998),

$$C_{IOM} = 0.049 * C_{tot,meas}^{1.139} \qquad (11)$$

where C_{IOM} is the C in the IOM pool (kg C ha^{-1});
$C_{tot,meas}$ is the measured total soil C (kg C ha^{-1}).

Next, a fraction of the remaining organic carbon, i.e. around 2% (Jenkinson and Coleman, 2008; Zimmermann et al., 2007), is attributed to the BIO pool, while the main part is comprised by the HUM pool.

Inputs of organic matter enter the soil as DPM and RPM for plant material (PM) with a fixed DPM/RPM ratio, i.e. 1.44 for agricultural crops (Coleman and Jenkinson, 1999), and also partially as HUM in case of manure. This ratio and the C:N ratio of the input material determine subsequently their respective C:N ratio, and thus determine the distribution of N to the PM pools. Mineral fertilizer is immediately assigned to the ammonium and/or nitrate pool depending of its composition. The plant material pools decompose into BIO and HUM with loss of C as carbon dioxide (CO_2). The BIO and HUM pools follow a feedback pathway which implies internal recycling. The decomposition of each pool and the parallel release of CO_2 might be restricted by rate modifiers due to changes in the environment:

$$\frac{dC_j}{dt} = fN_p * f_{DM} * \left(-k_j * C_j + \sum_{i=1}^{4} \alpha_{ji} * k_i * C_i\right) \qquad (12)$$

$$R_j = fN_p * f_{DM} * \frac{crat}{crat + 1} * k_j * C_j \qquad (13)$$

$$\alpha_{3i} = \frac{(B:BH)}{crat + 1} \quad \& \quad \alpha_{4i} = \frac{1 - (B:BH)}{crat + 1} \quad \& \; \alpha_{1i} = \alpha_{2i} = 0 \qquad (14)$$

$$crat = 1.67 * (1.85 + 1.6 * e^{-0.0786*clay}) \qquad (15)$$

where dC_j/dt is the change in carbon content of pool *j* per unit time (kg C ha^{-1} day^{-1});
R_j is the release of CO_2 out of pool *j* per day (kg CO_2-C ha^{-1} day^{-1});
fN_p and f_{DM} are rate limiting factors (-) in case of immobilisation: see equations (19) and (22);
k_j is the decay rate of the j^{th} pool (day^{-1});
α_{ji} is the dimensionless transfer coefficient of C from pool i to pool *j* (no recycling within the PM pools);
B:BH is the ratio of BIO to BIO+HUM (-);
crat is the ratio of CO_2 to BIO+HUM (-);
clay represents the percentage of clay in the soil layer (%).

The organic N content of the soil follows the decomposition of SOM-C in accordance with the fixed C:N ratio of the receiving pool. Maintaining this ratio determines if N is mineralized from SOM or immobilized from the mineral N pools favouring ammonium over nitrate.

$$\frac{dN_j}{dt} = fN_p * f_{DM} * \left(-k_j * N_j + \frac{\sum_{i=1}^{4} \alpha_{ji} * k_i * C_i}{C{:}N_j}\right) \tag{16}$$

$$MI_j = fN_p * f_{DM} * \left(k_j * N_j - \left(\frac{\alpha_{3i}}{C{:}N_3} + \frac{\alpha_{4i}}{C{:}N_4}\right) * k_j * C_j\right) \tag{17}$$

where dN_j/dt is the change in nitrogen content of pool *j* per unit time (kg N ha^{-1} day^{-1});
MI_j is the amount of N being mineralized from or immobilized to pool *j* per day (kg N ha^{-1} day^{-1});
$C{:}N_j$ is the C:N ratio (-) of the receiving j^{th} pool (i.e. BIO or HUM);
fN_p and f_{DM} are rate limiting factors (-) in case of immobilisation: see equations (19) and (22);
k_j is the decay rate of the j^{th} pool (day^{-1});
α_{ji} is the dimensionless transfer coefficient of C from pool i to pool *j* (no recycling within the PM pools, i.e. $\alpha_{1i} = \alpha_{2i} = 0$).

Potential mineralisation/immobilisation (MI_p) is calculated by summing equation (17) over all 4 pools, neglecting the term fN_p. Addition of organic material with a high C:N ratio can cause immobilisation of the soil mineral nitrogen by the BIO and HUM pool to maintain their fixed C:N ratio. First the NH_4^+ pool will be seized, followed by the NO_3^- pool when ammonium is exhausted. From the moment that also the nitrate supply does not meet the potential demand for all competing N processes to go through, potential decomposition and mineralisation will be limited by a mineral N availability factor *fNp*. The factor is a combined modifier of the ammonium (*amf*) and nitrate (*nif*) limiting factors, each of them assessed as the ratio of their respective content and incoming flows to the outgoing flows. If either *amf* or *nif* is 1, fN_p will become 1 as well. If mineralisation releases nitrogen to the NH_4^+ pool, i.e. no immobilisation is expected or $MI_p \geq 0$, fN_p is set to 1 and soil decomposition will not be limited. Yet, the latter does not prevent potential reduction of the outgoing flows from the mineral N pools by the respective availability factors *amf* and *nif*.

$$MI_a = fN_p * MI_p = amf * MI_p + nif * (MI_p - amf * MI_p) \tag{18}$$

or,

$$fN_p = \frac{MI_a}{MI_p} = \begin{cases} 1 & |\ MI_p \geq 0 \\ amf + nif - amf * nif & |\ MI_p \leq 0 \end{cases} \tag{19}$$

$$amf = min\left\{\begin{array}{ll}\dfrac{NH_4 + dN_{urea} + MI_p}{|-f_V * k_V * NH_4 - f_N * r_N|} & |\ MI_p \geq 0 \\ \dfrac{NH_4 + dN_{urea}}{|MI_p - f_V * k_V * NH_4 - f_N * r_N|} & |\ MI_p \leq 0\end{array} \quad ; \ 1\right\} \tag{20}$$

$$nif = min\left\{\begin{array}{ll}\dfrac{NO_3 + (1-a-c) * amf * f_N * r_N}{|-f_{DN} * r_{DN}|} & |\ MIp \geq 0 \\ \dfrac{NO_3 + (1-a-c) * amf * f_N * r_N}{|(1-amf) * MI_p - f_{DN} * r_{DN}|} & |\ MIp \leq 0\end{array} \quad ; \ 1\right\} \tag{21}$$

where MI_p is the aggregated potential mineralisation or immobilisation over all 4 pools (kg N ha^{-1} day^{-1});
MI_a is the actual or reduced amount of MI_p by the mineral N availability factor fN_p (-) in case of immobilisation (kg N ha^{-1} day^{-1});
amf and *nif* are the limiting mineral N availability factors regarding ammonium and nitrate respectively (-);
NH_4 is the ammonium content (kg N ha^{-1});
dN_{urea} is the incoming N flow per day from urea hydrolysis to the NH_4^+ pool if applicable (kg N ha^{-1} day^{-1}): see section 4.2.2;
k_V and r_N are the daily rates of outgoing flows of the NH_4^+ pool regarding ammonia volatilisation (NH_3) and nitrification respectively (day^{-1}) and possibly limited by the dimensionless rate modifiers f_V and f_N due to environmental conditions: see section 4.2.4 and 4.2.5;
NO_3 is the nitrate content (kg N ha^{-1});
a and c are the nitrification coefficients (-) that determine the proportions being emitted as the by-products *NO* and N_2O respectively: see section 4.2.5;
r_{DN} is the daily amount of nitrate as N being denitrified (kg N ha^{-1} day^{-1}) and possibly limited by the dimensionless rate modifier f_{DN} due to environmental conditions: see section 4.2.6.

Besides nitrogen availability, the SOM decay is also sensitive to temperature, soil moisture, crop cover and pH (Bradbury et al., 1993b; Smith et al., 1997) and the depth of the soil layer (Jenkinson and Coleman, 2008) through a dimensionless rate modifier f_{DM} (see also Figure 4-4):

$$f_{DM} = t_{DM} * m_{DM} * z_{DM} * cc_{DM} * a_{DM} \tag{22}$$

$$t_{DM} = \frac{47.9}{1 + e^{106/(T_a+18.3)}} \tag{23}$$

$$m_{DM} = \begin{cases} m_0 & | WC \le LL \\ 1-(1-m_0)*(TH-WC)/(TH-LL) & | LL < WC \le TH \\ 1 & | TH < WC \le FC \\ 1-(1-m_2)*(WC-FC)/(SAT-FC) & | FC < WC \le SAT \end{cases} \quad (24)$$

$$z_{DM} = \frac{-1/(1+e^{-dfs*(F-f)})}{-1/(1+e^{-dfs*(-f)})} \quad (25)$$

$$cc_{DM} = \begin{cases} 0.6 & | \; vegetation \\ 1 & | \; bare \end{cases} \quad (26)$$

$$a_{DM} = min\left\{a_{DM,min} + \left(1-a_{DM,min}\right) * \frac{pH - pH_{min}}{pH_{max} - pH_{min}} \;\; ; \;\; 1\right\} \quad (27)$$

where $t_{DM}, m_{DM}, z_{DM}, cc_{DM}$ and a_{DM} are the dimensionless rate modifiers that account for the impact of changes in temperature, moisture, soil layer depth, crop cover and pH respectively;
T_a is the average air temperature (°C);
WC, *LL*, *TH*, *FC* and *SAT* are the soil water content (cm^3 cm^{-3}) at current level, lower limit, threshold ($TH = LL + m_1 * (FC - LL)$), field capacity and saturation respectively;
m_0, m_1 and m_2 are the moisture rate modifiers at LL, TH and SAT (-);
F is the distance (cm) between the centres of the top layer and layer in question;
f is half of the top layer thickness (cm);
dfs is a depth factor (cm^{-1}) controlling the sigmoid decrease of decomposition rate as a function of depth;
$a_{DM,min}$ is the acidity rate modifier (-) that reduces decomposition to a minimum at a minimum pH;
pH_{max} is the critical threshold (-) below which the optimum rate starts to decreases to a minimum at pH_{min}, a minimum pH related to the site.

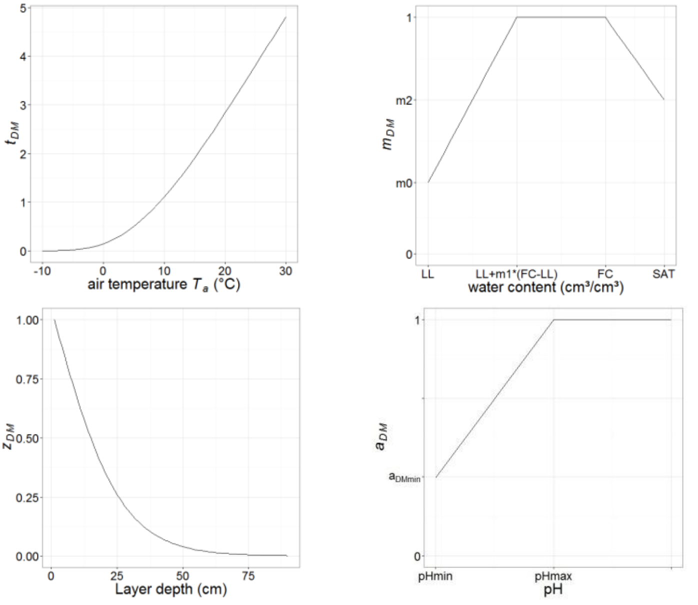

Figure 4-4 Decomposition rate modifiers due to changes in temperature, moisture, soil depth and pH.

4.2.2 Urea hydrolysis

First-order kinetics is also used for urea hydrolysis as applied by the CERES model (Jones and Kiniry, 1986) in case urea or urea-based fertilizers are applied to the soil. During urea hydrolysis, nitrogen is released to the ammonium pool and carbon dioxide is emitted with half the amount of nitrogen on a molar basis. The reaction rate k_H (i.e. potential hydrolysis fraction) with a minimum value of 0.25 is given by a regression equation based on organic carbon *OC* and pH, and sensitive to temperature and moisture variations (see also Figure 4-5).

$$\frac{dN_{Urea}}{dt} = -f_H * k_H * N_{Urea} \tag{28}$$

$$R_{Urea} = |0.5 * dN_{Urea}| \tag{29}$$

$$k_H = \max\{0.25\ ;\ -1.12 + 1.31 * OC + 0.203 * pH - 0.155 * OC * pH\} \tag{30}$$

$$0 \leq f_H = min\{t_H\ ;\ m_H\} = min\left\{\frac{T_s - T_m}{T_1 - T_m}\ ;\ m_{DM} + 0.2\right\} \leq 1 \tag{31}$$

where dN_{Urea}/dt is the change in nitrogen content of the applied urea per unit time (kg N ha^{-1} day^{-1});
R_{Urea} is the release of CO_2 per day (kg CO_2-C ha^{-1} day^{-1})
k_H is the reaction rate with modifier f_H
t_H is the temperature rate modifier determined by the soil temperature T_s, the minimum temperature T_m for which t_H is 0 and the temperature T_1 for which t_H is 1;
m_H is the moisture rate modifier similar to m_{DM}: see equation (24).

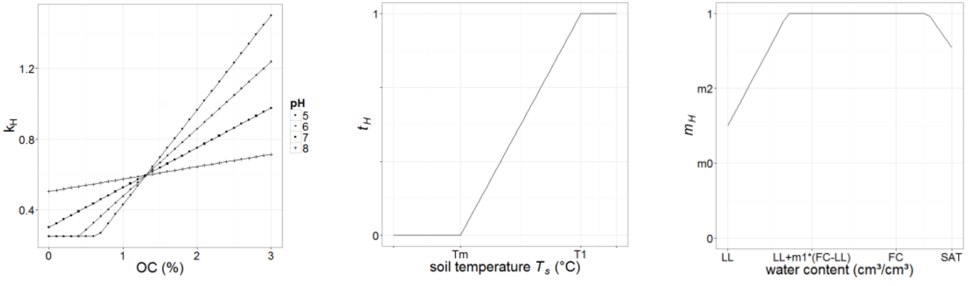

Figure 4-5 Urea hydrolysis rate (k_H) as a function of organic carbon content and pH of the soil; rate modifiers (t_H and m_H) due to changes in temperature and moisture.

4.2.3 Adsorption

Ammonium adsorption/desorption directly or indirectly affects the uptake of ammonium by plant roots, the buffering capacity of the soil for ammonium and the transformations of inorganic N in soil (Jia-Fang, 1997). Field observations imply that the role of adsorbed NH_4 in regulating soil N dynamics is not negligible. As commonly used, a Langmuir isotherm equation describes the partitioning between mobile ammonium in the soil solution (NH_4) and its adsorbed phase (N_{ADS}). In DNDC (Li et al., 2006) this was simplified under natural conditions to a linear adsorption isotherm equation in which the distribution coefficient *adsc* is expressed as a function of the cation exchange capacity (CEC) of the soil. The latter reflects the type and amount of clay minerals and organic matter content and complexes formed between them.

$$NH_4 = adsc * N_{ADS} \qquad (32)$$

$$adsc = a * e^{adsf*CEC} \qquad (33)$$

where NH_4 and N_{ADS} are the amounts of nitrogen as free ammonium in the soil solution and in its adsorbed form respectively (kg N ha^{-1});
adsc is the adsorption coefficient (-), determined by dimensionless empirical fitting constants *a* and *adsf*, and the cation exchange capacity *CEC* (cmol$_c$ kg^{-1}).

4.2.4 Ammonia volatilisation

The volatilisation of ammonia (NH_3) is known to be a major cause of soil-plant nitrogen loss and thereby counts as one of the largest sources of atmospheric ammonia pollution (Génermont and Cellier, 1997; Misselbrook et al., 2004). A first-order kinetic approach is applied with a rate constant k_V modified by a temperature factor f_V (Shaffer et al., 2001a; see Figure 4-6). Ammonia volatilisation is assumed to be relatively unaffected by soil pH given the neutral pH conditions for horticultural production in Flanders and the application of ammonium nitrate fertilizers. Harrison and Webb (2001) do suggest a reduction if ammonium sulphate or diammonium phosphate is applied and/or the soil is non-calcareous. Volatilisation is assumed to occur only at the top 15cm soil.

$$\frac{dNH_3}{dt} = amf * f_V * k_V * NH_4 \tag{34}$$

$$f_V = 1.68 * 10^9 * e^{\frac{-13}{1.99*10^{-3}*(T_{mod}+273)}} \tag{35}$$

where dNH_3/dt is the release of ammonia per unit time (kg N ha^{-1} day^{-1});
NH_4 is the ammonium soil content (kg N ha^{-1});
amf is the ammonium availability factor (-) assessed in equation (20);
k_V is the volatilisation rate (day^{-1});
f_V is the rate modifier regarding temperature (-);
T_{mod} is the soil temperature T_s (°C) until the optimum rate temperature of 30°C above which T_{mod} takes the value of $60 - T_s$.

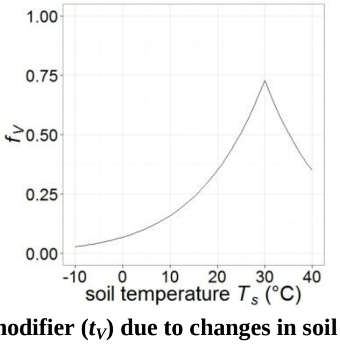

Figure 4-6 Volatilisation rate modifier (t_V) due to changes in soil temperature.

4.2.5 Nitrification

Under aerobic conditions ammonium is rapidly converted into nitrate with nitric and nitrous oxide (NO and N_2O respectively) as by-products. The submodule for this nitrification process is adapted from NOE2 (Bessou et al., 2010). It assumes that the nitrification rate depends on the ammonium level, soil temperature, water content and oxygen availability using the water filled pore space (WFPS, calculated as volumetric water content divided by the soil porosity) as an index of anoxia (see also Figure 4-7).

$$N_N = amf * f_N * PNR \tag{36}$$

$$f_N = n_N * t_N * min\{m_N \ ; \ O_{2,N}\} \tag{37}$$

$$n_N = \frac{NH_4^{\ *}}{NH_4^{\ *} + K_{nh4} * W} \tag{38}$$

$$t_N = e^{\frac{(T_s - 20) * \ln(Q_{10n})}{10}} \tag{39}$$

$$0 \leq \ m_N = \frac{W - a_W * FC/BD}{(1 - a_W * FC/BD} \ \leq 1 \tag{40}$$

$$O_{2,N} = a_s * \frac{WFPS - 1}{WFPS - b_s} \tag{41}$$

Where N_N is the daily amount of ammonium being nitrified and added to the nitrate pool (kg N ha^{-1} day^{-1});
PNR is the potential nitrification rate (kg N ha^{-1} day^{-1});
amf is the ammonium availability factor (-) assessed in equation (20);
f_N is the rate modifier (-) which combines the dimensionless response factors to ammonium N content (n_N), to temperature (t_N), to moisture (m_N) and to direct oxygen availability ($O_{2,N}$);
NH_4* is the ammonium N content (mg N kg^{-1});
W is the gravimetric water content (kg water kg^{-1}soil);
K_{nh4} is the half saturation constant (mg N L^{-1} water);
T_s is the soil temperature (°C);
FC is the water content at field capacity (cm^3 cm^{-3} soil);
BD is the soil bulk density (g/cm^3);
WFPS is the water filled pore space (-);
Q_{10n} *(=3.17)*, a_W *(=0.3)*, a_s *(1.16)* and b_s (=1.09) are empirical constants (-).

The fraction of N_2O emitted per unit of nitrified N (N_N) depends on WFPS, while the fraction of NO is kept constant.

$$N_2O_N = c * N_N \tag{42}$$

$$NO_N = a * N_N \tag{43}$$

$$c = c_0 * \frac{c_s * WFPS - d_s}{WFPS - d_s} \tag{44}$$

where N_2O_N and NO_N are the daily amounts of N in their respective form emitted from soil during nitrification (kg N ha^{-1} day^{-1});
a and c are the proportion coefficients (-), for the latter with dimensionless empirical constants c_s (=0.4) and d_s (=1.04).

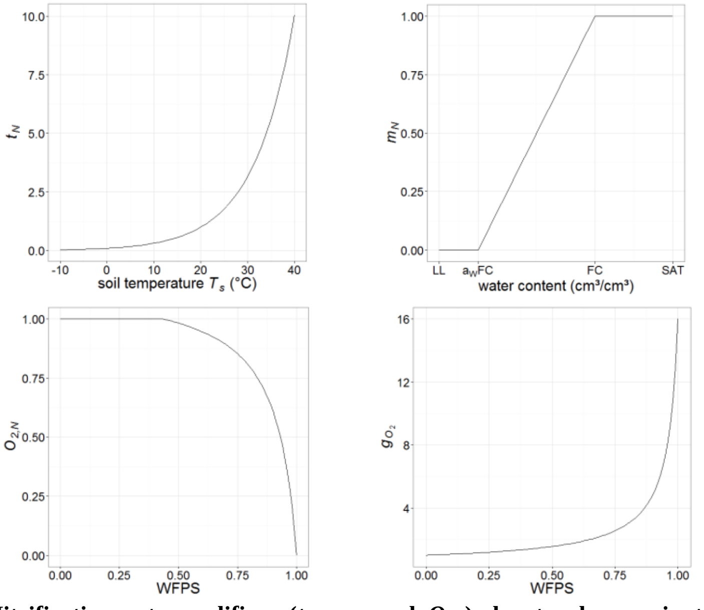

Figure 4-7 Nitrification rate modifiers (t_N, m_N and O_{2N}) due to changes in temperature, moisture and anoxia (WFPS) respectively, as well as the effect of anoxia on the amount of N_2O formed during nitrification (g_{O2}).

4.2.6 Denitrification

During denitrification nitrate is reduced to N_2 which occurs in poorly aerated soil conditions. Compared to nitrification, the release of NO tends to be very small as it is highly reactive under these conditions, while N_2O is emitted by a significant larger amount (Bessou et al., 2010). In the model, the rate of denitrification is assumed to depend on nitrate content and affected by temperature and moisture content (see also Figure 4-8) according to the following equations from Bessou et al. (2010):

$$N_{DN} = nif * f_{DN} * PDR \tag{45}$$

$$f_{DN} = n_{DN} * t_{DN} * m_{DN} \tag{46}$$

$$n_{DN} = \frac{NO_3{}^*}{NO_3{}^* + K_{no3} * W} \tag{47}$$

$$t_{DN} = \begin{cases} e^{\frac{(T_S-11)*\ln(Q_{10d1})-9*\ln(Q_{10d2})}{10}} & | \; T_s < 11 \\ e^{\frac{(T_S-20)*\ln(Q_{10d2})}{10}} & | \; T_s \geq 11 \end{cases} \tag{48}$$

$$m_{DN} = \begin{cases} 0 & | \; WFPS < WFPS_C \\ \left(\frac{WFPS - WFPS_C}{1 - WFPS_C}\right)^{1.74} & | \; WFPS \geq WFPS_C \end{cases} \tag{49}$$

Where N_{DN} is the daily amount of nitrate being denitrified to N_2 (kg N ha^{-1} day^{-1});
PDR is the potential denitrification rate (kg N ha^{-1} day^{-1});
nif is the nitrate availability factor (-) assessed in equation (21);
f_{DN} is the rate modifier (-) which combines the dimensionless response factors to nitrate N content (n_{DN}), to temperature (t_{DN}) and to moisture;
NO_3^* is the nitrate N content (mg N kg^{-1});
W is the gravimetric water content (kg water kg^{-1}soil);
K_{no3} is the half saturation constant (mg N L^{-1} water);
T_s is the soil temperature (°C);
Q_{10nd1} *(=89)* and Q_{10nd2} *(=2.1)* are temperature coefficients;
$WFPS_C$ is the threshold water filled pore space (-) below which denitrification does not occur.

Denitrified N is partitioned into N_2O and end product N_2 using simple linear functions which depends on WFPS and nitrate content.

$$N_2O_{DN} = r * nif * N_{DN} \tag{50}$$

$$N_2 = (1 - r) * nif * N_{DN} \tag{51}$$

$$r = r_0 * G_{O_2} * G_{DN} \tag{52}$$

$$G_{O_2} = 1 - c_W * max\{0;\; WFPS - WFPS_C\} \tag{53}$$

$$G_{DN} = min\{d_{N0} * NO_3\;;\;\; c_N + d_N * NO_3\;;\;\; 1\} \tag{54}$$

where N_2O_{DN} and N_2 are the daily amounts of N in their respective form emitted from soil during denitrification (kg N ha^{-1} day^{-1});
r is the proportion coefficient (-) with a maximum value of r_0 *(=0.63)* and dimensionless response factors to respectively WFPS (G_{O_2}) and nitrate concentration (G_{DN});
c_W *(=2.05)*, d_{N0} *(=0.148)*, c_N *(=0.44)* and d_N *(=0.0015)* are empirical coefficients that determine the linear relation.

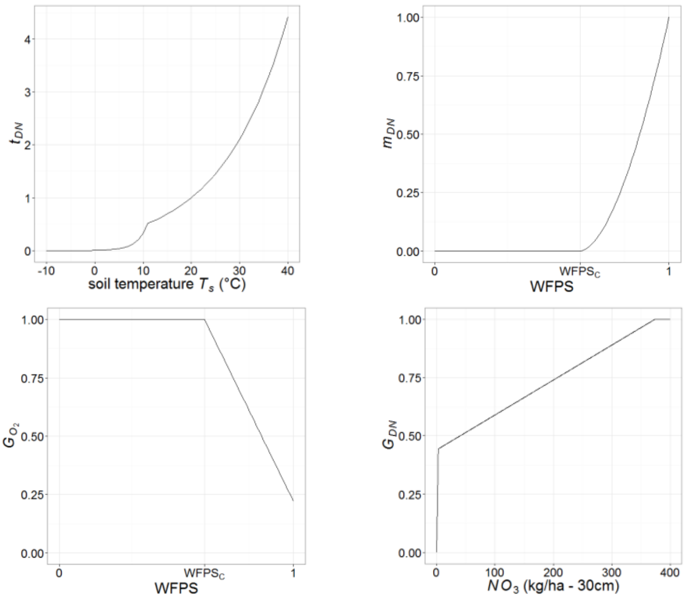

Figure 4-8 Denitrification rate modifiers (t_{DN} and m_{DN}) due to changes in temperature and moisture, as well as the effect of anoxia (WFPS) and nitrate content on the partitioning of denitrified N into N_2O and N_2 (G_{O2} and G_{DN}).

4.3 Interception submodel

Water from rainfall and irrigation may be partially intercepted by vegetation where it is stored on leaves, branches and stems. The amount of water reaching the soil decreases with increasing vegetation cover. Merriam (1960) proposed a relationship which included an exponential term to consider gross rainfall. Based on the data of Aston (1979) rain interception has to be further reduced to prevent overestimation accounting for the canopy throughfall or leaf density given the current LAI (de Jong and Jetten, 2007a). The maximum rain detention is characterised by the canopy storage capacity (S_{max}) which is related to the LAI based on the analysis of a series of crops by von Hoyningen-Huene (1984).

$$I = SC_{max} * (1 - e^{-\frac{k*P}{SC_{max}}}) \tag{55}$$

$$k = 0.065 * LAI \tag{56}$$

$$SC_{max} = 0.935 + 0.498 * LAI - 0.00575 * LAI^2 \tag{57}$$

where I is the daily amount of intercepted water (cm);
P is the daily rainfall (cm)
k is a correction factor for canopy throughfall (-);
LAI is the leaf area index (m^2 leaf surface m^{-2} ground surface);
SC_{max} is the maximum canopy storage capacity (cm);

As suggested by Šimůnek et al. (2013), the water intercepted by the canopy is considered to evaporate back to the atmosphere which reduces the potential plant transpiration as calculated in the evapotranspiration model (section 4.7 equation (98)).

4.4 Runoff submodel

Surface runoff may occur when the amount of water that reaches the soil (i.e. not intercepted) exceeds the infiltration capacity of the soil. The NRCS Curve Number (CN) method is empirical but widely applied due to the availability of CN values in soil maps and databases. It estimates the daily surface runoff (*RO*) accounting for the hydraulic properties of soil, land use, slope and soil moisture content (USDA-NRCS, 2004). This procedure is applied daily to the top soil layer.

$$RO = \frac{(P_{ni} - I_a)^2}{P_{ni} - I_a + S} \quad | \, P_{ni} > I_a \tag{58}$$

$$I_a = C_{I_a} * S \tag{59}$$

$$S = 2.54 * \left(\frac{1000}{CN} - 10\right) \tag{60}$$

where RO is the daily amount of surface runoff (cm);
P_{ni} is the rainfall (including irrigation) that is not intercepted by vegetation (cm);
I_a is the initial abstractions which include the initial amount of surface storage, interception and infiltration that is retained prior to runoff (cm);
C_{I_a} is the initial abstraction ratio estimated by a regression coefficient depending on the vegetation, land use and site condition;
S is the site storage index or retention parameter (cm) for a given day depending on the soil conditions which is transformed to the curve number CN.

The curve number, however, is a function of the soil's permeability, land use and antecedent soil water conditions. The NRCS introduced the Antecedent Runoff Condition (ARC) to describe the factors causing CN variability. ARC is divided into three classes of runoff conditions. For dry (*I*) or wet (*III*) conditions, equivalent curve numbers can be computed with the CN number for average moisture conditions (*II*) as follows (Tarboton, 2003):

$$CN_I = \frac{4.2 * CN_{II}}{10 - 0.058 * CN_{II}} \tag{61}$$

$$CN_{III} = \frac{23 * CN_{II}}{10 + 0.13 * CN_{II}} \tag{62}$$

Neitsch et al. (2011) proposed a new equation under average conditions which is implemented to make the retention parameter *S* change with soil characteristics and soil moisture content (see also Figure 4-9).

$$S = \begin{cases} S_I & | \, SWC \leq LL \\ S_I * (1 - \dfrac{sw * LT}{sw * LT + e^{w_1 - w_2 * sw * LT}}) & | \, LL \leq SWC \leq SAT \\ 0.254 & | \, SWC \geq SAT \end{cases} \tag{63}$$

$$w_1 = \ln\left(\frac{fc * LT}{1 - S_3/S_1} - fc * LT\right) + w_2 * fc * LT \tag{64}$$

$$w_2 = \frac{\ln\left(\dfrac{fc}{1 - S_3/S_1} - fc\right) - \ln\left(\dfrac{sat}{1 - 2.54/S_1} - sat\right)}{(sat - fc) * LT} \tag{65}$$

where S_i is the retention parameter (cm) calculated in equation (60) using the curve number CN_i under the dry (*i*=I) or wet (*i*=III) condition as calculated in equations (61) and (62) respectively;
sw, *fc* and *sat* are respectively the current soil water content *SWC*, the water content at field capacity *FC* and water content at saturation level *SAT* excluding the content at lower limit *LL* ($cm^3\ cm^{-3}$)
LT is the layer thickness *LT* (cm);
w_1 and w_2 are the shape coefficients (-) under the assumption that *S* equals S_I, S_{III} and 0.254 for moisture contents at respectively lower limit (*LL*), field capacity (*FC*) and saturation (*SAT*).

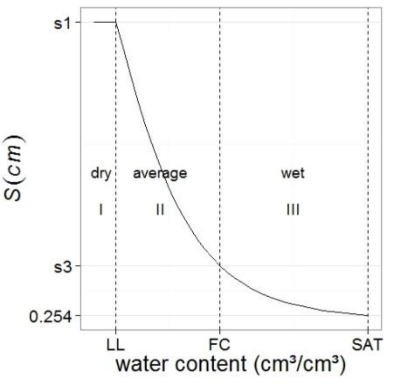

Figure 4-9 The soil retention parameter (*S*) for the ARC (Antecedent Runoff Conditions) classes *I, II* and *III* related to the soil water content at lower limit (*LL*), field capacity (FC) and saturation (SAT).

Furthermore, the curve number under average conditions (CN_{II}) is assigned by the NRCS to four hydrologic soil groups based on their runoff potential and assumes a 5% slope and initial abstraction ratio (C_{I_a}) of 0.2. Their values are adjusted for a different slope (i.c. zero slope) according to Sharpley and Williams (1990) and for a different C_{I_a} of 0.05 as suggested by Woodward et al. (2003).

$$CN_{IIs} = \frac{CN_{III} - CN_{II}}{3} * \left(1 - 2 * e^{-13.86 * slp}\right) + CN_{II} \qquad (66)$$

$$CN_{0.05} = \frac{100}{0.153 * \left(\frac{1000}{CN_{0.2}} - 10\right)^{1.15} + 1} \; or \; S_{0.05} = 1.53 * S_{0.2}^{1.15} \qquad (67)$$

where CN_{IIs} is the moisture condition II curve number (-) adjusted for an average fraction slope *slp* (-);
$CN_{0.05}$ and $CN_{0.2}$ are the curve numbers (-) for an initial abstraction ratio of respectively 0.05 and 0.2, along with the transformed equation regarding the corresponding retention parameter *S* (cm).

The runoff curve concept was empirically derived to approximate the runoff volume when only daily rainfall is known. If a greater accuracy is required, a more physically based approach would be required (Tsuji et al., 1998).

4.5 Drain submodel

Due to gravitational forces, water above field capacity drains or percolates to the lower soil layer. This component of soil water dynamics thereby transports soluble nutrients as ammonium and nitrate which may lead to leaching into the groundwater causing a eutrophic burden to the environment. The drainage submodule is based on the cascade or 'tipping bucket' approach from Burns (BURNS, 1974) and CERES, adapted in DSSAT (Jones et al., 2003). This one-dimensional model computes daily changes in soil water content by soil layer as well as the amount of nitrogen (i.e. ammonium and nitrate) which are transferred along due to vertical drainage. Potential downward water flow W_p (cm) for each layer *l* with thickness *LT* consist of oversaturated flow W_d (i.e. excess water above saturation *SAT*) and saturated flow *DRAIN* (i.e. drainage).

$$W_{p,l} = W_{d,l} + DRAIN_l \tag{68}$$

where $W_{p,l}$ is the potential downward flow (cm) from layer *l*;
$W_{d,l}$ is the oversaturated flow (cm);
$DRAIN_l$ is the saturated flow (cm).

First the oversaturated flow is calculated if the incoming flow from the layer above (or rainfall for the top layer, adjusted for interception and runoff) exceeds its saturated holding capacity. This amount is immediately distributed to the next layer and the soil water content SWC_l is adjusted accordingly.

$$W_{d,l} = \max\{0\ ;\ W_{p,l-1} - (SAT_l - SWC_l) * LT_l\} \tag{69}$$

$$SWC_l = \min\left\{SWC_l + \frac{W_{p,l-1}}{LT_l}\ ;\ SAT_l\right\} \tag{70}$$

where $W_{d,l}$ is the oversaturated flow (cm) of layer *l*;
$W_{p,l-1}$ is the potential downward flow (cm) from the layer *l-1* above;
SAT_l and SWC_l are the soil water contents ($cm^3\ cm^{-3}$) at saturation limit and current state respectively;
LT_l is the layer thickness (cm) of layer *l*.

Secondly, if the adjusted water content exceeds the water content at field capacity FC_l, the saturated flow (*DRAIN*) is calculated with the soil water conductivity (*SWCON*), i.e. drainage rate coefficient as a function of the soil porosity and field capacity.

$$DRAIN_l = \max\{0\ ;\ SWCON_l * (SWC_l - FC_l) * LT_l\} \tag{71}$$

$$SWC_l = SWC_l - \frac{DRAIN_l}{LT_l} \tag{72}$$

$$SWCON_l = \frac{\varphi_l - FC_l}{\varphi_l} \ \& \ \varphi_l = 1 - \frac{BD_l}{2.65} \tag{73}$$

where $DRAIN_l$ is the amount of saturated flow (cm);
$SWCON_l$ is the soil water conductivity (day^{-1}) or drainage rate constant;
LL_l, SWC_l , FC_l and SAT_l are the water contents (cm³ cm^{-3}) at lower limit, current state, field capacity and saturation respectively;
LT_l is the layer thickness (cm) of layer *l*;
φ_l is the soil layer porosity (-) with an assumed particle density of 2.65 g cm^{-3};
BD_l is the soil layer bulk density (g cm^{-3}).

Due to the constant drainage rate per day and the decreasing soil water content in the soil layer, the drainage follows an exponential decay over time. The movement of nitrogen for each layer is assumed to be proportional to the water flow and its initial content.

$$Z_{p,l} = \frac{W_{p,l}}{W_{p,l} + SWC_l * LT_l} \tag{74}$$

$$W_{N,l} = Z_{p,l} * (N_l + W_{N,l-1}) \tag{75}$$

$$N_l = N_l + W_{N,l-1} - W_{N,l} \tag{76}$$

where $Z_{p,l}$ is the fraction of water moved from layer *l* to the next, representing as well the fraction of nitrogen transported along (-);
$W_{p,l}$ is the potential downward flow (cm) from layer *l*;
SWC_l *is* the current soil water content (cm³ cm^{-3});
LT_l is the layer thickness (cm) of layer *l*;
$W_{N,l}$ is the amount of nitrogen as ammonium and nitrate (kg N ha^{-1}) being transported along with the water flow;
N_l is the nitrogen content (NH_4^+ or NO_3^-) in each soil layer (kg N ha^{-1}).

The amount of water and within the dissolved ammonium and nitrate lost from the bottom layer are considered as leached from the soil profile (i.e. deep percolation).

4.6 Crop submodel

For both cauliflower and leek growth a phenological compartmentation model is developed (Figure 4-10) based on TOMGRO (Jones et al., 1989) . The main part of each crop module is similar, as it is a generic approach that might be adapted for other crops to be incorporated. Differences per crop are stated at the separate model components. After initialisation concerning the seedling characteristics, the simulation is accomplished through evaluating 1) the crop developmental stage (DVS), 2) gross photosynthesis and maintenance and growth respiration, 3) biomass growth (as dry matter) and its partitioning into growing organs, 4) leaf area and 5) the crop organs nitrogen demand. All of these processes are dynamic and affected by environmental (climate and soil) and cultivar specific factors. Each crop module includes crop specific information to predict the variations in plant ontogeny and yield component characteristics and their interactions with climate. The crop growth starts at planting date with given seedlings characteristics, i.e. dry matter (DM) of the plant organs, initial leaf area and root depth as well as the plant density. Calculations are done on a per plant basis unless specified otherwise. Two time loops are applied with a daily time increment for the main loop which integrates an hourly loop for photosynthesis and respiration.

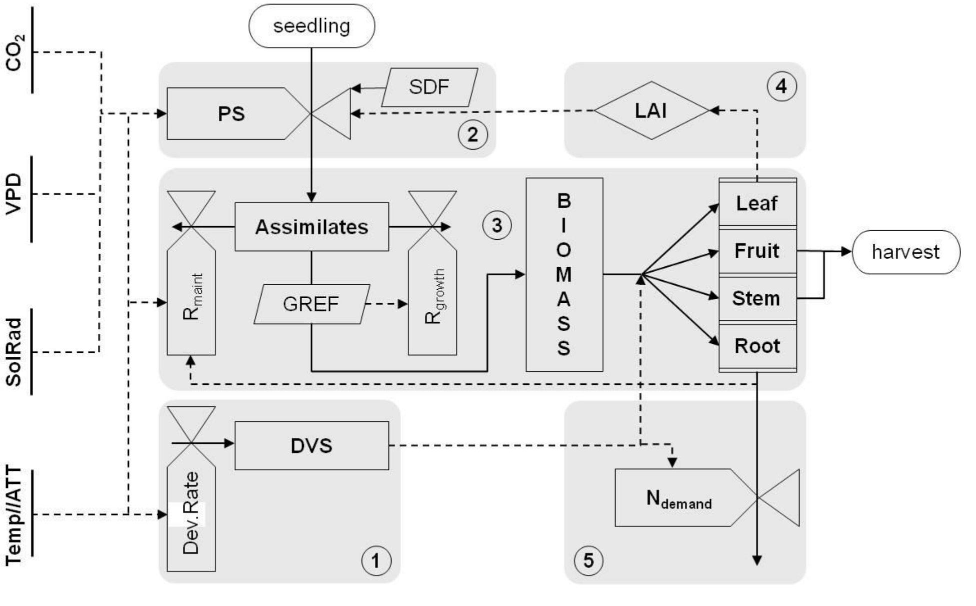

Figure 4-10 Flowchart of the crop growth module: boxes, valves and diamonds represent state, rate and auxiliary variables; lines are flows of matter (solid) or information (dashed); others are in- and output data.

The DVS or the crop phenological state is driven primarily from the air temperature and it affects the allocation rate from the structural biomass pool to the different plant organs. With the concept of accumulated thermal time (*ATT*), developmental phases of the crop, assigned by a number, are directly related to daily accumulations of positive air temperature above a certain base temperature below which physiological activity is assumed inhibited. The DVS of leek evolves from 0 at seedling stage to 1 at maturity or harvestable form, while cauliflower growth is characterized by two phases, with DVS evolving from 0 at seedling phase over 1 at curd initiation until 2 at maturity (see also Figure 4-11).

$$DVS_i = \begin{cases} DVS_{01,i} = min\left\{\frac{ATT_i}{ATT_1}\ ;\ 1\right\} & leek \\ DVS_{01,i} + DVS_{12,i} = min\left\{\frac{ATT_i}{ATT_1};1\right\} + min\left\{\frac{ATT_i - ATT_1}{ATT_2};1\right\} & cauliflower \end{cases} \quad (77)$$

$$ATT_i = \sum_{d=1}^{i} T_{ef,d} * (1\ day) \quad with \quad T_{ef,d} = T_d - T_b \quad (78)$$

where DVS_i is the developmental stage of the crop at day i;
ATT_i is the accumulated thermal time (degree days) at the end of day i or effective temperature integrated over time from planting date ($d=1$) until current day i;
ATT_1 and ATT_2 are the calibrated thermal time thresholds to reach DVS 1 (curd initiation for cauliflower, maturity for leek) and DVS 2 (maturity for cauliflower) respectively, both reset at zero at beginning of the respective phase;
$T_{ef,d}$ is the effective temperature on day d, i.e. average day temperature (T_d) corrected for a base temperature (T_b) of the crop.

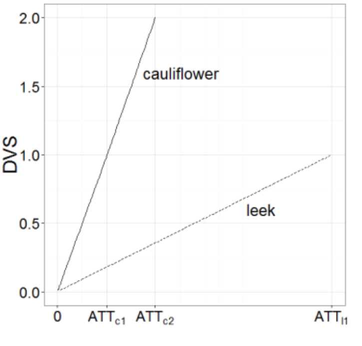

Figure 4-11 Developmental stage (*DVS*) for both cauliflower and leek growth as a function of thermal time ATT with corresponding thresholds at curd initiation (ATT_{c1} for cauliflower) and maturity (ATT_{c2} for cauliflower & ATT_{l1} for leek).

Both crops are harvested right before inflorescence emergence, i.e. reaching for cauliflower a sufficiently grown curd and for leek a satisfactory shaft (stem) length and diameter. Leaf senescence (unit less correction factor), specific leaf area (SLA, $cm^2\ g^{-1}$), biomass compartmentation over different organs and N-demand of different organs (%) are changing in relation to DVS.

Through Acock *et al.*'s submodel (1978), gross photosynthesis ($P_{g,h}$) is computed hourly for the whole canopy whereby the total leaf area captures solar radiation and CO_2.

$$P_{g,h} = \frac{P_{max}}{X_K} * \ln\left(\frac{(1 - X_m) * P_{max} + Q_e * X_K * PPFD}{(1 - X_m) * P_{max} + Q_e * X_K * PPFD * e^{-X_K * LAI}}\right) \quad (79)$$

$$P_{max} = \tau * CO_2 * PGRED * PDVS * PVPD \quad (80)$$

where $P_{g,h}$ is the gross photosynthesis per unit ground area (µmol $CO_2\ m^{-2}s^{-1}$);
X_K and X_M are the respective light extinction and transmission coefficient (-) in the canopy;
Q_e is the light use efficiency (µmol CO_2 mol^{-1} photon);
PPFD is the photosynthetic photon flux density or radiation intensity above the canopy (mol photons $m^{-2}s^{-1}$);
LAI is the leaf area index (-);
P_{max} is the maximum leaf photosynthesis rate (µmol $CO_2\ m^{-2}s^{-1}$) corrected for suboptimal temperatures, leaf senescence and air vapour pressure deficit by respectively dimensionless factors *PGRED*, *PDVS* and *PVPD*, respectively (Figure 4-12);
τ is the CO_2 use efficiency ($m\ s^{-1}$);
CO_2 is the ambient CO_2 concentration (µmol $CO_2\ m^{-3}$air).

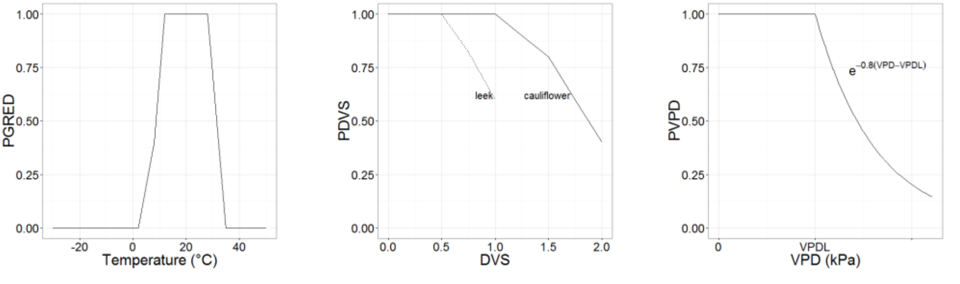

Figure 4-12 Correction functions reducing photosynthesis at suboptimal temperatures (PGRED), leaf senescence (PDVS) and high vapour pressure deficit (PVPD) respectively.

Integration over the day with unit conversion results in daily gross photosynthesis per plant (P_g).

$$P_g = \sum_{h=1}^{24} \left(P_{g,h} * 3600\right) * \frac{30 * 10^{-6}}{PLD} \tag{81}$$

where P_g is the gross photosynthesis per plant (g CH_2O plant^{-1} day^{-1})
PLD is the plant density (plants m^{-2});
3600 is the number of seconds per hour;
30 is the molecular weight of CH_2O (g mol^{-1});
10^{-6} is a scaling factor from µmol to mol.

Through a feedback mechanism the occurrence of stress conditions (lack of water and/or nutrients compared to the crop demand) is accounted for by adjusting photosynthesis by a soil deficiency factor (*SDF*) which will limit the potential dry matter accumulation and subsequently the LAI which lowers potential plant transpiration and the nutrient demand. SDF is the minimum of the two deficiency factors from the Uptake modules (sections 4.8.1 and 4.8.2). This implies that in case of stress this crop growth submodel is run twice that day:

1. representing the potential growth with SDF=1 and
2. the actual growth accounting for the real SDF factor

Crop growth is driven by the accumulation of net carbon assimilated by leaves and transformed into biomass, i.e. plant dry matter (DM_p), accounting for maintenance respiration (R_m,) which is proportional to plant mass and corrected for temperature using a Q_{10} value (Jones et al., 1989; Penning de Vries, 1975).

$$DM_p = \left(P_g - R_m\right) * SDF * GREF \tag{82}$$

$$R_m = \left(RMR_l * \left(TDM_{(G)L} + TDM_S\right) + RMR_f * TDM_C\right) * Q_{10}^{0.1*(T-T_{ref})} \tag{83}$$

where DM_p is the daily dry matter increase (g DM plant^{-1} day^{-1});
P_g and R_m are the daily photosynthesis and respiration respectively (g CH_2O plant^{-1}day^{-1});
GREF is the growth efficiency (g DM g^{-1} CH_2O) due to extra loss through growth respiration;
SDF is the soil deficiency factor (-) due to water and/or nitrogen stress (see Uptake submodule section 4.8);
TDM_{GL}, TDM_S and TDM_C are the total dry matter of the (green) leaves, stem and curd (in case of cauliflower) respectively (g DM plant^{-1})
RMR_l and RMR_f are respiration coefficients (g CH_2O g^{-1} DM) for the corresponding plant organs;

Q_{10} is the factor by which the respiration rate increases for every 10-degree rise in temperature;
T is the air temperature (°C);
T_{ref} is the reference temperature for which the respiration parameters are given.

The partitioning of this biomass into the various plant organs (leaves, stems, roots and fruits) evolves according with the phenological development. Roots are grown daily in a fixed proportion to the above ground production or shoot.

$$DM_X = \frac{Xf}{1 + Rf} * DM_p \tag{84}$$

$$Rf = min \left\{ \frac{Rf_{sh}}{SDF} \;\; ; \;\; 1 \right\} \tag{85}$$

where DM_X is the daily dry matter increase of the plant organ X (g DM plant^{-1} day^{-1}), i.e. L, S, C and R for respectively (dead & green) leaves, stem, curd (in case of cauliflower) and roots;
Xf is the dry matter fraction of the plant organ X;
Rf_{sh} is the constant root to shoot ratio (-).

Equation (85) assures that in case of stress (SDF<1), the assimilates go preferentially to the roots.
In case of cauliflower, leave senescence occurs resulting in dead leaf dry matter after reaching a threshold developmental stage (DVS_{th}).

$$DM_{DL} = \left(e^{K_d(\sim T_{ef})} - 1\right) * DM_L \;\; | \;\; DVS \geq DVS_{th} \tag{86}$$

where DM_{DL} is the dry matter increase of dead leaves (g DM plant^{-1} day^{-1});
DM_L is the dry matter increase of leaves, dead and green (g DM plant^{-1} day^{-1});
K_d is the dead leaf fraction coefficient as a function of the effective temperature (T_{ef}).

Dry matter accumulation of the different plant organs brings along important plant characteristics for further growth and related processes. As the leaf grows, the leaf area of the plant increases according to the specific leaf area (SLA) as a function of DVS. SLA quantifies the increment of leaf area per unit of leaf dry matter. Subsequently the leaf area index (LAI) or ratio of leaf area to soil area changes altering the photosynthetic capacity as well as the evapotranspiration (see section 4.7).

$$LAI = TotLeafArea * PLD \tag{87}$$

$$TotLeafArea = SLA(\sim DVS) * TDM_{GL} \tag{88}$$

where LAI is the leaf area index at the current day (m² leaf m² ground);
PLD is the plant density (plants m^{-2});
TotLeafArea is the total accumulated leaf area (m²) at the current day since planting;
SLA(~DVS) is the specific leaf area (m² leaf g^{-1} leaf DM) as empirically estimated as a function of DVS;
TDM_{GL} is the total accumulated dry matter (g DM $plant^{-1}$) of green leaves since planting.

Furthermore, the root dry matter will be distributed according to a virtual distribution (see section 4.8.1) over the rooting depth (*RD*), the latter being simulated with a logistic function for cauliflower and linear for leek (see also Figure 4-13).

$$RD = \begin{cases} RD_{ini} + \dfrac{RD_{max} - RD_{ini}}{1 + 8.83 * (e^{-5.9*DVS})^{1/0.45}} & \mid cauliflower \\ RD_{ini} + \dfrac{RD_{max} - RD_{ini}}{ATT_{l1}} * ATT_{l1} & \mid leek \end{cases} \tag{89}$$

Where RD_{ini} and RD_{max} are the initial and maximum rooting depths (cm);
ATT_{l1} is the accumulated thermal time at leek maturity or DVS 1. Above DVS 1 for cauliflower and above ATT_{l1} for leek, roots are not supposed to grow anymore.

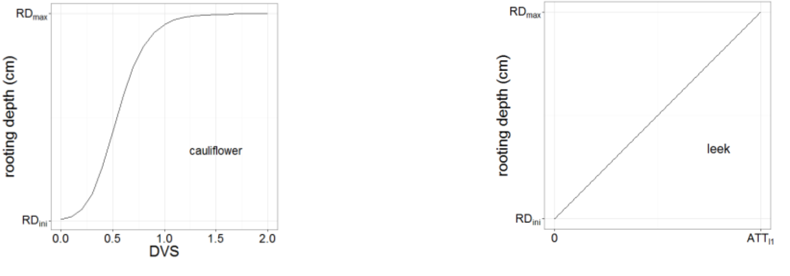

Figure 4-13 Rooting depth evolution of cauliflower and leek as a function of DVS and thermal time respectively.

For leek, additionally, shaft dimensions are simulated as a function of thermal time as length (*ShaftLe*) and diameter (*ShaftDi*) are quality measures and determine the time of harvest (Figure 4-14). The exponential relation was fitted on observed data during the experiments.

$$ShaftDi = e^{2.24 + r_{di} * ATT} \tag{90}$$

$$ShaftLe = e^{2.06 + r_{le} * ATT} \tag{91}$$

where r_{di} and r_{le} are the growth rates of the shaft diameter and length respectively (cm °C^{-1}day^{-1}).

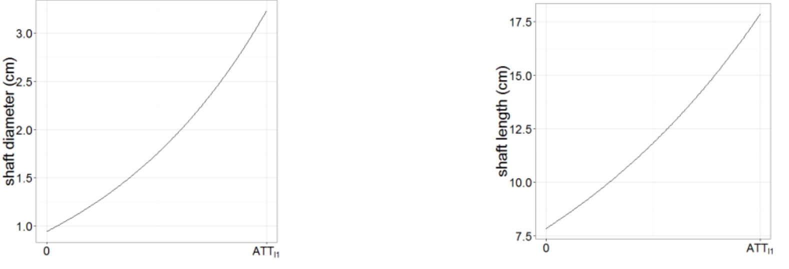

Figure 4-14 Shaft dimensions, i.e. diameter and length as a function of thermal time.

Among the essential nutrients, nitrogen is the most required by the plant due to its involvement in photosynthesis and proteins related to cell division and plant growth. As such it can also limit growth if insufficient amounts are available for uptake from the soil (see above and section 4.8.2). The crop N demand is defined on a dry matter basis with a critical N concentration function. The latter corresponds to the minimum N concentration permitting maximal crop growth and generally declines as the plant develops, i.e. with increasing DVS (Jeuffroy et al., 2002).

$$N_X = X_{Nc}(\sim DVS) * DM_X / 100 \tag{92}$$

where N_X is the N demand of plant organ X (g N plant^{-1} day^{-1}) with X being L, S, C and R for respectively (dead & green) leaves, stem, curd (in case of cauliflower) and roots ;
X_{Nc} is the critical N concentration (%) of the organ as a function of DVS;
DM_X is the dry matter increase of the plant organ X (g DM plant^{-1} day^{-1}).

The crop N demand, summed over all organs, will be compared, given a unit conversion, in the nitrogen uptake model (see section 4.8.2 equation (109)) with the N supply in the soil to check if stress is expected and crop growth has to be limited.

4.7 Evapotranspiration submodel

Critical to the water status of soil and plant is the loss of water through soil evaporation and plant transpiration. The potential crop evapotranspiration (ET_c) is calculated using the ASCE Standardized Reference Evapotranspiration equation (ET_0) based on the commonly used Penman-Monteith equation (Allen et al., 1998) which is based on an energy balance for an evaporating surface and incorporates aerodynamic and surface resistance terms.

$$ET_c = K_c * ET_0 \tag{93}$$

$$ET_0 = \frac{0.408 * \Delta * (R_n - G) + \gamma * \frac{c_1}{T_a + 273.16} * u_2 * VPD}{\Delta + \gamma * (1 + c_2 * u_2)} \tag{94}$$

where ET_c is the potential crop evapotranspiration (mm day^{-1});
ET_0 is the reference evapotranspiration for a grass surface (mm day^{-1});
K_c is the crop coefficient (-) which integrates the effects of characteristics that distinguish the cropped surface from the reference one;
Δ is the rate of change of the saturated vapour pressure with air temperature (kPa °C^{-1});
R_n is the net radiation at crop surface (MJ m^{-2} day^{-1});
G is the soil heat flux density (MJ m^{-2} day^{-1});
γ is the psychrometric constant (kPa °C^{-1}) based on the altitude;
T_a is the mean daily air temperature (°C);
c_1 and c_2 are constants as a function of time step and resistance (i.e. reference crop type, short or tall);
u_2 is the wind speed at 2m height (m s^{-1});
VPD is the saturation vapour pressure deficit (kPa) based on temperature and relative humidity.

This stand-alone method lacking LAI is combined with the approach of Dejonge et al. (2012) which defines a crop coefficient (K_c) as a function of LAI to obtain the ET_c concept (DeJonge et al., 2012; Sau et al., 2004), see also Figure 4-15.

$$K_c = K_{c,ini} + \left(K_{c,max} - K_{c,ini}\right) * (1 - e^{-K_{c,lai} * LAI}) \tag{95}$$

Where K_c is the crop coefficient (-);
$K_{c,ini}$ is the initial crop coefficient (-) at LAI=0;
$K_{c,max}$ is the maximum crop coefficient (-) at high LAI:
$K_{c,lai}$ is a shape parameter that determines the shape of the K_c versus LAI curve (Figure 4-15 left).

As for a bare soil or in the initial vegetation period, the effect of evaporation is predominant and ET is sensitive to the top soil water status. Therefore the $K_{c,ini}$ is adjusted for the relative water content through an exponential equation that accounts for a sharp decline in hydraulic conductivity with decreasing water content (Raes et al., 2009).

$$0 \leq K_r = \frac{e^{f_K * WC_r} - 1}{e^{f_K} - 1} \leq 1 \tag{96}$$

where K_r is the dimensionless reduction coefficient applied on $K_{c,ini}$ which assumes a wet soil;
WC_r is the relative water content (-), i.e. the ratio of soil water content to saturated water content;
f_K is a decline factor (-).

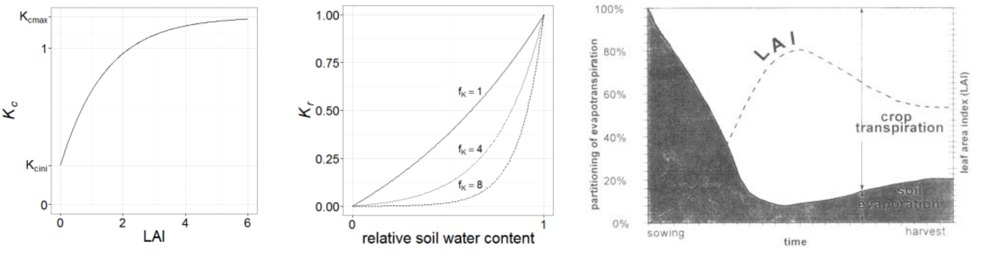

Figure 4-15 Left: Variation of crop coefficient K_c as a function of LAI; middle: the effect of the relative soil water content for bare soils and initial vegetation stages; right: the partitioning of ET into soil evaporation and plant transpiration over the vegetation period

Based on the crops' LAI ET_c is partitioned into potential soil evaporation (SE_p) and potential plant transpiration (PT_p) with the latter being reduced by potential intercepted water by the crop canopy.

$$SE_p = ET_c * e^{-KEP*LAI} \tag{97}$$

$$PT_p = ET_c * (1 - e^{-KEP*LAI}) - I \tag{98}$$

Where SE_p is the potential soil evaporation (mm day^{-1});
PT_p is the potential plant transpiration (mm day^{-1});
ET_c is the potential crop evapotranspiration (mm day^{-1})
KEP is an energy extinction partitioning coefficient (-) of the canopy for total solar irradiance which is related with but not directly taken from the light extinction coefficient used for PAR (Sau et al., 2004): see section 0 equation (79);
I is the intercepted water (mm day^{-1}): see section 4.3 equation (55).

The potential demand of plant transpiration is further translated in actual soil water uptake in the submodule of root water uptake (section 4.8.1). Actual soil evaporation is calculated in the submodule of evaporation (section 0) to check if the potential rate can be met as well mainly depending on the soil water availability.

4.8 Uptake submodel

An adequate supply of water and nutrients is one of the most important resources required for plant growth. Their uptake by roots is the result of a complex process controlled by soil, plant and atmospheric conditions. To simplify, a one-dimensional root length density (RLD) profile is applied based on the CERES model (Jones and Kiniry, 1986) which assumes a homogeneous root architecture and horizontal root growth. Therefore it only requires root dry matter and rooting depth, besides current water and nitrogen contents in the rooted soil layers.

4.8.1 Water uptake

In order to vertically determine the root water uptake, the daily newly formed root dry matter is partitioned over the rooting depth according to a relative distribution function within the soil profile. Based on sampled rooting data, as addressed in section 2.2.3 and explained by Vansteenkiste et al. (2014), mapping the rooting depth and relative distribution allowed the elaboration of a virtual root distribution function similar to a set of root form parameters (Pedersen et al., 2010), but less complex. This distribution function relates root dry matter fractions to a virtual rooting depth (Figure 4-16). The root length density can then be calculated in order to assess the actual root water uptake in each soil layer as follows:

$$RLD_{l,i} = \left(TDM_{R,l,i-1} + DM_R * RDPF_l(\sim RD_i)\right) * \frac{SRL * PLD}{LT_l * 10000} \quad (99)$$

where $RLD_{l,i}$ is the root length density (cm cm^{-3}) in layer l at the current day i;
$TDM_{R,l,i-1}$ is the total root dry matter (g DM plant^{-1}) in soil layer l from the previous day $i-1$;
DM_R is the increase of root dry matter (g DM plant^{-1} day^{-1});
$RDPF_l\ (\sim RD_i)$ is the root distribution factor (-) for layer l as a function of the rooting depth RD at day i;
SRL is the specific root length (cm g^{-1});
PLD is the plant density (plants m^{-2});
LT_l is the layer thickness (cm).

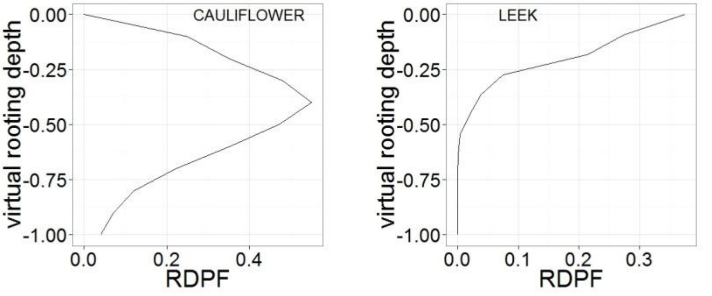

Figure 4-16 The relative root distribution function to partition the dry matter over the rooted layers from the initial root depth (for leek at the base of the shaft) to the current rooting depth.

Subsequently the 'law of the limiting' approach of the microscopic CERES model as used by DSSAT was applied (Jones and Kiniry, 1986; Jones et al., 2003). It is an approximation to the radial flow equation, where assumptions are made about soil texture effect on hydraulic conductivity, root diameter and a maximum water potential difference between roots and the soil. Maximum daily water uptake by roots in a layer has been determined by trial and error to be 0.03cm³ water cm^{-1} root. It is also assumed that the water potential gradient between the root and soil remains constant. The water uptake in all rooted layers depends on the soil water content and root length density as follows.

$$0 \leq RWUP_l = \frac{swcon_1 * e^{min\{swcon_{2,l}*(SWC_l - LL_l);\ 40\}}}{swcon_3 - \ln{(RLD_l)}} \leq RTWU_m \tag{100}$$

$$swcon_2 = max\{45\ ;\ 120 - 250 * LL_l\} \tag{101}$$

$$RWUPLa_l = RWUP_l * RLD_l * LT_l \tag{102}$$

where $RWUP_l$ and $RWUPLa_l$ are the daily root water uptake amounts in layer *l* per unit root length ($cm^3\ cm^{-1}$ root day^{-1}) and per unit area ($cm^3\ cm^{-2}$ or cm day^{-1}) respectively;
$RTWU_m$ is the maximum plant limited flow rate ($cm^3\ cm^{-1}\ day^{-1}$);
$swcon_{1,3}$ are empirically derived constants (-) in determining root water uptake accounting for root and soil resistance;
$swcon_{2,l}$ is a variable constant (-) dependent on the lower limit in layer *l* with a minimum value of 45*;*
SWC_l and LL_l are the respective current and lower limit soil water content ($cm^3\ cm^{-3}$) of layer *l*;
RLD_l is the root length density ($cm\ cm^{-3}$) of layer *l*;
LT_l is the layer thickness (cm).

Whether the potential transpiration is met and water stress may occur is captured by a water uptake factor *WUF*. If the total possible water uptake (i.e., summed over the rooted layers) exceeds the potential transpiration, the water uptake rate for each rooted layer is reduced proportionally with *WUF*.

$$WUF = \frac{\sum_l RWUPLa_l}{PT_p} \tag{103}$$

where WUF is the water uptake factor (-);
$RWUPLa_l$ is the root water uptake in layer l (cm day^{-1});
PT_p is the potential plant transpiration (cm) as calculated in section 4.7 by equation (98) adjusted for unit conversion from mm to cm.

If the summed amount of water however does not meet the potential demand (i.e. potential transpiration), water stress is assumed (see Table 4-1). Water uptake in each rooted layer and thus actual transpiration is limited to the maximum water availability ($RWUPLa_l$), while a soil water deficit factor (*SWDF*) equals the water uptake factor and is passed to the crop module again to restrict the daily dry matter growth.

Table 4-1 Effect of water stress on root water uptake

NO water stress	Water stress	
$SWFD = 1$	$SWFD = WUF$	
$RWU_l = \frac{RWUPLa_l}{WUF}$	$RWU_l = RWUPLa_l$	(104)
$PT_a = PT_p$	$PT_a = \sum_l RWUPLa_l$	

where $SWDF$ is the soil water deficit factor (-);
WUF is the water uptake factor (-);
RWU_l is the actual daily root water uptake (cm day^{-1}) from layer l;
$RWUPLa_l$ is the root water uptake in layer l (cm day^{-1});
PT_p and PT_a are the potential and actual plant transpiration (cm).

The water content in each rooted layer is ultimately adjusted for its actual water loss by subtracting the root water uptake accounting for the layer thickness.

$$SWC_l = SWC_l - \frac{RWU_l}{LT_l} \tag{105}$$

where SWC_l is the soil water content ($cm^3\ cm^{-3}$) in layer l;
RWU_l is the actual daily root water uptake (cm day^{-1}) from layer l;
LT_l is the layer thickness (cm).

4.8.2 Nitrogen uptake

Like above, actual nitrogen uptake is assessed according to the nitrogen uptake model in DDSAT (Jones and Kiniry, 1986) by comparing the potential supply of N in the soil with the daily N demand from the crop. Potential uptake of nitrogen by the plant is calculated for both ammonium and nitrate. They are sensitive to the rooting density, the soil water content and their respective nitrogen concentration.

$$RNUP_l = RLD_l * SMDFR_l^2 * LT_l * 100 * FN_l * RTN_m \tag{106}$$

$$SMDFR_l = \begin{cases} \dfrac{SWC_l - LL_l}{FC_l - LL_l} & \mid SWC_l \leq FC_l \\ 1 - \dfrac{SWC_l - FC_l}{SAT_l - FC_l} & \mid SWC_l > FC_l \end{cases} \tag{107}$$

$$FN_l = min\{1 - e^{-af*SN_l} \;;\; 1\} \tag{108}$$

where $RNUP_l$ is the daily amount of ammonium or nitrate (kg N ha^{-1} day^{-1}) that can be taken up from layer l;
RTN_m is the maximum uptake of ammonium or nitrate per unit root length (mg N cm^{-1} root day^{-1});
RLD_l is the root length density (cm cm^{-3}) in layer l;
$SMDFR_l$ and FN_l are the soil moisture and nitrogen (ammonium or nitrate) availability factors (-);
SN_l is the soil nitrogen concentration of ammonium or nitrate (mg N kg^{-1});
af is a nitrogen availability coefficient (-) for ammonium or nitrate.

Similar to the water uptake, a nitrogen uptake factor (NUF) is defined as the ratio of the total potential nitrogen supply in the rooted soil to the nitrogen demand from the plant.

$$NUF = \frac{\sum_l RNUP_l}{Ndem_p * PLD * 10} \tag{109}$$

where NUF is the nitrogen uptake factor (-);
$RNUP_l$ is the daily amount of ammonium or nitrate (kg N ha^{-1} day^{-1}) that potentially can be taken up from layer l;
$Ndem_p$ is the potential N demand from the crop (g N plant^{-1} day^{-1}) as calculated by the sum of equation (92) over all organs: see section 0;
PLD is the plant density (plants m^{-2});

Nitrogen uptake will be reduced if the total potential nitrogen (ammonium and nitrate) supply or potential uptake from the rooted soil layers exceeds the N demand from the crop (see Table 4-2). The total root nitrogen uptake will amount to the nitrogen demand of the plant. When nitrogen stress does occur, i.e. NUF<1 or the supply is not sufficient to meet the demand, NUF determines the soil nitrogen deficit factor (*SNDF*). In that case, the actual uptake, summed over the soil layers, will be limited to the potential uptake available in the rooted layers and *SNDF* is passed to the crop module through the feedback loop restricting the biomass growth of that day.

Table 4-2 Effect of nitrogen stress on root nitrogen uptake

No nitrogen stress	Nitrogen stress	
$SNDF = 1$	$SNDF = NUF$	
$RNU_l = \frac{RNUP_l}{NUF}$	$RNU_l = RNUP_l$	(110)
$\sum_l RNU_l = Ndem_p$	$\sum_l RNU_l = \sum_l RNUP_l$	

where *SNDF* is the soil nitrogen deficit factor (-);
NUF is the nitrogen uptake factor (-);
RNU_l is the actual daily root nitrogen (ammonium or nitrate) uptake (kg N ha^{-1} day^{-1}) from layer *l*;
$RNUP_l$ is the daily amount of ammonium or nitrate (kg N ha^{-1} day^{-1}) that potentially can be taken up from layer *l*;
$Ndem_p$ is the potential N demand from the crop (g N plant^{-1} day^{-1}).

Ultimately, if the supply does not meet the demand, either for water and/or nitrogen, the minimum of both factors *SWDF* and *SNDF* is passed on to the 'global' soil deficiency factor *SDF* that reduces dry matter accumulation which will be calculated again by equation (82) (section 0). Therefore, the model returns to the consecutive submodules for crop growth (section 0) and evapotranspiration (section 4.7), which will result in a reduced dry matter accumulation, LAI, crop N demand and transpiration that correspond with the actual supply under stress conditions.

4.9 Evaporation submodel

As plant transpiration can be limited due to limited water availability, the latter can also reduce the potential soil evaporation determined in the evapotranspiration module (section 4.7). An extended diffusion based model for soil water evaporation (Ritchie et al., 2009) is applied that describes upward water flow by a power relation as a function of soil depth (see also Figure 4-17).

$$SE_{av,l} = F_l * (SWC_l - SWEF_l * LL_l) * LT_l \tag{111}$$

$$F_l = a_l * z_l^{(b_l)} \tag{112}$$

$$SWEF_l = 0.9 - 0.00038 * (LT_l - 30)^2 \tag{113}$$

$$a_l = \begin{cases} 0.26 \\ 0.011 \\ 0.5 + 0.24 * FC_l \end{cases} \quad \& \quad b_l = \begin{cases} -0.7 & |\, wet \\ 0 & |\, equilibrium \\ -2.04 + 0.2 * FC_l & |\, dry \end{cases} \tag{114}$$

where $SE_{av,l}$ is the available amount of water to evaporate daily from soil layer l (cm day^{-1});
F_l is the upward flow or transfer coefficient (day^{-1}) at depth z of layer l;
SWC_l and LL_l are the current soil water content and at lower limit respectively (cm³ cm^{-3}) in layer l;
LT_l is the layer thickness (cm);
z_l is the mean depth (cm) of layer l;
$SWEF_l$ is the soil water evaporation factor (-) adjusting the lower limit LL until which the soil can dry out;
a_l and b_l are empirical coefficients (-) developed according to the diffusion theory (Figure 4-17).

Three profile type conditions, each with a different set of transfer coefficients are referred to as

1. wet, when the upper layers have the highest water contents,
2. equilibrium, when the lower layers have water content above field capacity with constant water transfer, and
3. dry, when the soil water contents in all layers are below FC.

In order to determine the current condition, a threshold water content is defined for transitioning between wet and equilibrium conditions.

$$SWC_{eq} = 0.257 * FC_1 + 1.165 * FC_1^2 + 1.2 * z_1 * FC_1^{3.75} \tag{115}$$

where SWC_{eq} is the threshold water content (cm³ cm^{-3});
FC_1 is the soil water content at field capacity (cm³ cm^{-3});
z_1 is the mean depth of the top layer (cm).

This threshold will decide between a wet or equilibrium condition when the soil water content is above FC in at least one layer in the top 100 cm. When all these soil layers contents are at or below FC, the coefficients for 'dry' conditions are applied.

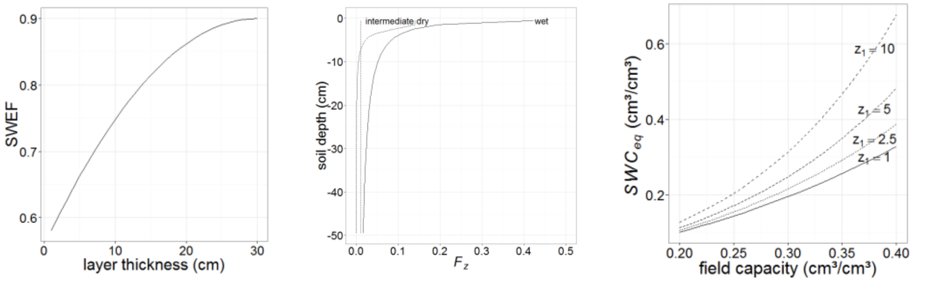

Figure 4-17 Adjustment factor SWEF lowering the lower limit until which evaporation can dry out the soil; the upward flow coefficient F_z as a function of soil depth; and the threshold soil water content between wet and equilibrium condition as a function of *FC* and mean depth z_1 of top layer.

Ultimately, the actual soil evaporation per layer is limited to the available amount possibly reduced if the total available water for evaporation (SE_{av}) exceeds the potential demand (SE_p). Actual soil evaporation is then levelled with the potential. If SE_p is not met by SE_{av}, actual evaporation equals the available amount as the reduction factor *RedFac* is limited to one.

$$SE_{a,l} = SE_{av,l} * RedFac \tag{116}$$

$$RedFac = \frac{SE_p}{\sum_l SE_{av,l}} \leq 1 \tag{117}$$

$$SWC_l = SWC_l - \frac{SE_{a,l}}{LT_l} \tag{118}$$

where $SE_{a,l}$ and $SE_{av,l}$ are the actual and available amounts of water that evaporate daily (cm day^{-1}) from layer *l*;
RedFac is the ratio of potential soil evaporation (SE_p: see section 4.7 equation (97)) to the total available amount that can be evaporated from all the soil layers;
SWC_l is the soil water content (cm³ cm^{-3}) of layer *l*;
LT_l is the layer thickness (cm).

Finally, the soil water contents of each layer are updated according to equation (118) by subtracting the actual evaporated water.

4.10 Diffusivity submodel

Soil evaporation and water uptake by plants create hydraulic gradients and, as a consequence, water flow will occur between adjacent layers until they reach hydraulic equilibrium. Following the approach in DSSAT (Hoogenboom et al., 2015), the model calculates the flow between two adjacent layers by multiplying a soil water content gradient with a diffusivity that depends on the average soil water content of two adjacent layers normalized to lower limit.

$$FLOW_{l,p} = DBAR * GRAD \tag{119}$$

$$DBAR = min\left\{0.88 * e^{\left(35.4 * \frac{\theta_l * LT_l + \theta_{l+1} * LT_{l+1}}{LT_l + LT_{l+1}}\right)} \; ; \; 100\right\} \tag{120}$$

$$GRAD = \frac{\left(\frac{\theta_{l+1}}{ESW_{l+1}} - \frac{\theta_l}{ESW_l}\right) * \left(\frac{ESW_l * LT_l + ESW_{l+1} * LT_{l+1}}{LT_l + LT_{l+1}}\right)}{(LT_l + LT_{l+1}) * 0.5} \tag{121}$$

$$ESW_l = FC_l - LL_l \quad \& \quad \theta_l = SWC_l - LL_l \tag{122}$$

where $FLOW_{l,p}$ is the daily potential water flow (cm day^{-1}) out of (negative) or into (positive) layer *l*;
DBAR is the water diffusivity (cm² day^{-1}) that applies for the flow between layers *l* and *l+1* and is limited to 100 cm² day^{-1};
GRAD is the gradient (cm³ cm^{-3} cm^{-1}), i.e. the ratio of the difference of the normalized soil water contents between the adjacent layers to the distance of the soil layer centres;
θ_l is the soil water content (SWC_l, cm³ cm^{-3}) of layer *l* normalized to lower limit (LL_l);
ESW_l is the extractable amount of water (cm³ cm^{-3}) available in layer *l*;
LT_l is the layer thickness (cm).

The actual flow is restricted to unsaturated flow such that new soil water levels remain between lower limit and field capacity.

$$FLOW_{l,a} = \begin{cases} max\left\{FLOW_{l,p} \; ; \; -\theta_l * LT_l ; \; -(FC_{l+1} - SWC_{l+1}) * LT_{l+1}\right\} & | \; (-) \\ \min\left\{FLOW_{l,p} \; ; \theta_{l+1} * LT_{l+1} ; (FC_l - SWC_l) * LT_l\right\} & | \; (+) \end{cases} \tag{123}$$

where $FLOW_{l,a}$ is the daily actual water flow (cm day^{-1}) out of (negative) or into (positive) layer l;
$FLOW_{l,p}$ is the daily potential water flow (cm day^{-1}) out of (negative) or into (positive) layer l;
θ_l is the current soil water content (SWC_l) of layer l normalized to lower limit (LL_l) (cm³ cm^{-3});
FC_l is the soil water content at field capacity (cm³ cm^{-3}) of layer l;
LT_l is the layer thickness (cm).

The movement of water, upwards or downwards, carries along the dissolved nitrogen. Subsequently the ammonium and nitrate contents as well as the water content of each soil layer are updated accordingly with the respective amounts. The following calculations are done for both ammonium and nitrate.

$$Z_{c,l} = \begin{cases} \dfrac{FLOW_{l,a}}{SWC_l * LT_l} & |(-) \\ \dfrac{FLOW_{l,a}}{SWC_{l+1} * LT_{l+1}} & |(+) \end{cases} \quad \& \quad W'_{N,l} = \begin{cases} Z_{c,l} * N_l & |(-) \\ Z_{c,l} * N_{l+1} & |(+) \end{cases} \tag{124}$$

$$N_l = N_l + W_{N,l} \quad \& \quad N_{l+1} = N_{l+1} - W_{N,l} \tag{125}$$

$$SWC_l = SWC_l + \frac{FLOW_{l,a}}{LT_l} \quad \& \quad SWC_{l+1} = SWC_{l+1} - \frac{FLOW_{l,a}}{LT_{l+1}} \tag{126}$$

where $Z_{c,l}$ is the fraction of water moved out of (-) or into (+) layer l, representing as well the fraction of nitrogen transported along;
$FLOW_{l,a}$ is the daily actual water flow (cm day^{-1}) out of (negative) or into (positive) layer l;
SWC_l is the soil water content (cm³ cm^{-3}) of layer l;
LT_l is the layer thickness (cm);
$W'_{N,l}$ is the corresponding amount of nitrogen (NH_4 or NO_3) transferred along (kg N ha^{-1});
N_l is the nitrogen (NH_4 or NO_3) content (kg N ha^{-1}) in layer l .

Chapter 5. Model calibration & sensitivity

In order to predict crop growth, soil water and nitrogen fluxes accurately, the model should perform well under different conditions regarding the environment and/or management of the system. The first step was the calibration procedure which involved a sensitivity analysis to assess key parameters. Their precision required consecutively a manual or automatic calibration. The integrated model was calibrated with observed data during the cauliflower – leek rotation of 2009 treated with the reference N dose (N dose 3) through broadcast application (cf. Chapter 2). Once the model output corresponded closely to the field observations, as well graphically as quantitatively, the next step consisted of the model validation with independent data from the 2 subsequent year rotations and the 3 other nitrogen dose applications (see Chapter 6).
The calibration of the model implied parameters to be adjusted either based on field data or in line with information found in literature. Sensitivity analysis was the process of determining the rate of change in model output to changes in model inputs or parameters. It allowed the assessment of acceptable intervals for parameter values to match the simulated output to field observations regarding changes in soil water and nitrogen content as well as soil temperature. No water or nitrogen stress was assumed to occur during crop growth under the reference N dose 3 rate, so crop biomass and its nitrogen content reached their observed values. The reliability of the calibrations depends partly on the quality and quantity of the input data. Parameters were adjusted further by reasoned trial and error until the best possible fit was obtained.
In first instance the crop module was calibrated separately for both crops assuming there was no limitation of water nor nitrogen. This involved the DVS calculation with the observed timing of curd initiation for cauliflower and maturity for both crops, with the corresponding accumulated thermal time. Subsequently, tabulated functions were implemented for leaf area expansion, plant organ compartmentation, cauliflower leaf senescence and critical N content in relation to the accumulated thermal time and corresponding DVS. Next, once the LAI and plant N demand were calibrated, the other modules were integrated with the crop module and calibrated such that potential crop growth under the reference N dose 3 rate was reached and the simulated soil water and mineral nitrogen contents approached the observations as close as possible regarding the propagation over time and the performance statistics. Actual water and nitrogen uptake should meet the potential plant transpiration and N demand respectively.
Although certain parameters could not be calibrated per se with the measurements from the experiment, literature values were implemented and presented here as they (in)directly affect the interaction with the processes and variables that were observed.
The model performance is graphically displayed and quantified with different statistical indicator variables presented in Table 5-3. Subsequently, the results of

the sensitivity analysis are presented regarding the effect of fixed changes to the most significant and relevant key parameters on the output corresponding to the calibration results.

5.1 Model input

Unlike the model parameters, the following main input data is considered fixed and comprises simulation control settings, climate conditions, soil profile properties and crop management including irrigation and fertilizer application as stated in the model description (see Chapter 4). These were all observed or specified during the experiments.

5.1.1 Simulation control settings

The reference date (*RefDate*) for the simulation was set at 1 January 2009. The simulation started at 3 March 2009 (*NSTART*), the planting date of the cauliflower and ended at 17 March 2010, 379 days (*NDAYS*) later when the next rotation cycle started. Regarding geographical settings, the altitude was set at 5 m. The latitude and longitude of the experimental setup was 51.1°N and 4.5°E respectively.

5.1.2 Climate

Climate data for the respective submodules of the model included hourly solar radiation, precipitation, relative humidity, air temperature and wind speed, which were collected during the experiment. Recordings during the first crop rotation are presented in Figure 5-1. Solar radiation that reached the surface daily varied from 0.4 MJ m^{-2} until 29.2 MJ m^{-2}. It is a key governing factor for crop growth and evapotranspiration processes. A total of 731 mm of rain fell with almost 60% in March and from October on while an occasionally intensive event in July. The average daily air temperature varied between -8.2 and 24.7°C with August and January being the warmest and coldest month of the cycle. The average relative humidity ranged from 51.2 till 91.1%. Average wind speed maintained 1.6 m s^{-1} over the full cycle.

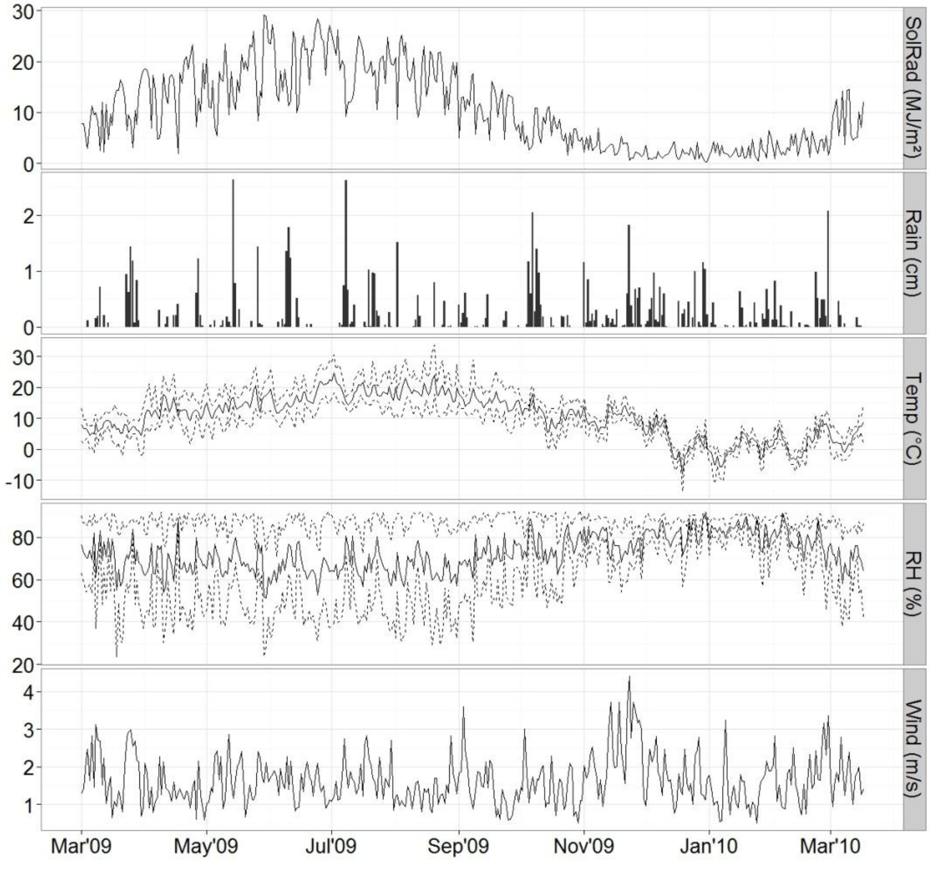

Figure 5-1 Climate input (daily) for calibration year 2009 including relative humidity (RH, %), precipitation or rain (cm), solar radiation (SolRad, MJ m^{-2}), air temperature (Temp, °C) and wind speed (Wind, m s^{-1}). Dashed lines represent daily minimum and maximum values regarding humidity and temperature.

5.1.3 Soil profile properties

In accordance with the soil observations made during the experiments, the soil profile was divided into 4 layers (0-10, 10-30, 30-60 and 60-90cm), with the two top layers having the same characteristics except for layer thickness. The depth increment of each layer needs to be sufficiently small to accommodate the functional simulation procedures needed to reasonable predict the water status. In general, the values of layer thickness (*LT*) should not exceed about 20cm near the surface and 30 cm for deeper depths (Ritchie, 1998). Most soil characteristics like texture, pH, organic carbon content (*OC*) and cation exchange capacity (*CEC*) were measured through soil analysis at the start of the experiment. The soil water characteristics at different thresholds, i.e. at lower limit (*LL*), at field capacity (*FC*) and at saturation (*SAT*) were estimated by fitting the function of van Genuchten (1980) on experimental data. These moisture retention characteristics were measured on undisturbed 100cm³ ring samples using a suction table (sand box) for lower pressures and a pressure plate extractor (Soil moisture Equipment Corp.) for higher pressures (Dane and Hopmans, 2002). Initial contents of water (*SWC*) and nitrogen (*N*) were measured as described in the experimental setup (see Chapter 2). All these properties are summarized in Table 5-1.

Table 5-1 Soil physical and chemical data for the profile collected at the start of calibration year 2009 (Layer thickness (LT), soil bulk density (BD), soil water content at lower limit (LL), field capacity (FC), saturation (SAT) and initial level (SWC)).

Layer	LT [cm]	BD [g/cm³]	LL [cm³/cm³]	FC [cm³/cm³]	SAT [cm³/cm³]	SWC [cm³/cm³]
1	10	1.4	0.07	0.29	0.46	0.32
2	20	1.4	0.07	0.29	0.46	0.32
3	30	1.5	0.06	0.33	0.44	0.32
4	30	1.6	0.04	0.33	0.40	0.33

Table 5-1 (Continued) Soil physical and chemical data for the profile collected at the start of calibration year 2009 (soil salinity (pH), soil organic carbon content (OC), soil mineral nitrogen content (N_{min}), cation exchange capacity(CEC) and texture share of clay, silt and sand)

Layer	pH	OC [%]	N_{min} [kg/ha]	CEC [$cmol_c$/kg]	Clay [%]	Silt [%]	Sand [%]
1	7.0	1.6	6.2	10	8	28	64
2	7.0	1.6	9.3	10	8	28	64
3	6.2	1.1	10.2	8	7	23	70
4	6.2	0.2	10.2	5	7	28	65

5.1.4 Crop management

The current crop growth model does not include the nursery phase from seed till seedling. Yet, it starts after transplanting which requires initial values for the seedlings characteristics. Furthermore, extra culture technical information is needed as mentioned in the model description. In order for the crop to grow, the supply of water and nitrogen additional to the soil contents, was provided through irrigation and fertilizer application respectively.

Crop characteristics

The planting dates of cauliflower and leek were the 3rd of March and 25th of June in 2009 with a planting density of 4 and 18.18 plants m^{-2} respectively. The characteristics of the seedlings from both crops are presented as well in Table 5-2. It includes dry matter of their plant organs (leaf, stem and curd; the root dry matter is estimated unless measurements are available), the maximum rooting depth, initial specific leaf area (SLA_i) and the base temperature (T_b) below which plant growth ceases. The latter is accounted for during estimation of the crop development stage (*DVS*) in relation to the accumulated thermal time (*ATT*, see section 0). For calibration procedure this also required the harvesting dates as well as the date of curd initiation during cauliflower growth. DVS in relation to ATT and days after planting is shown in Figure 5-2. Cauliflower reached maturity in 90 days after 671 degree days with curd initiation after 59 days or 341.3 degree days. Leek was harvested after 132 days when 1881.9 degree days were reached from its planting date.

Table 5-2 Overview crop characteristics and management input from the experiment in 2009 required for the model calibration.

		Unit	Cauliflower	Leek
Planting		-	3/03/2009	25/6/2009
Curd initiation		-	1/05/2009	-
Harvesting		-	1/06/2009	4/11/2009
Planting density		Plants m^{-2}	4	18.18
ATT		degree days	671	1881.9
ATT_1 (DVS 1)			341.3	1881.9
ATT_2 (DVS 2)			329.7	-
Cultivation length		days	90 (59+31)	132
Dry matter	Leaf	g	0.28	1.96
	Stem	g	0.15	0.35
	Root	g	0.04	0.2
Initial specific leaf area		$cm^2\ g^{-1}$	195	95
Base temperature		°C	4 (Olesen and Grevsen, 1997)	2 (Baumann et al., 2002)

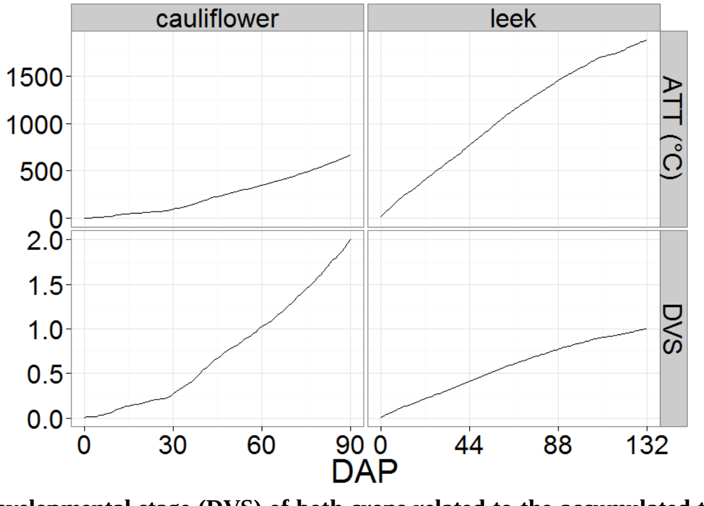

Figure 5-2 Developmental stage (DVS) of both crops related to the accumulated thermal time (ATT) as a function of days after planting (DAP).

Irrigation and fertilizer application

Regarding irrigation, the daily amount was specified. In 2009 additional water was applied at the planting of leek and during warm days in August and September to compensate limited precipitation and/or meet the expected plant transpiration demand. The irrigation scheme as well as the fertilizer application is presented in Figure 5-3.

Fertilizer management requires time of application, soil depth incorporation, amounts (kg C or N ha^{-1}) and the CN ratio in case of organic inputs like crop residues or manure. Based on the broadcast application of N dose 3, i.e. the reference dose, three applications of inorganic fertilizer were applied on the soil surface: 130 and 25 kg N ha^{-1} at the start of cauliflower cultivation and respectively 7 weeks later and 100 kg N ha^{-1} 5 weeks after the leek planting date. One week after cauliflower harvest, incorporation of its crop residue with a CN ratio of 12.7 added 1166 kg C ha^{-1} and 91.8 kg N ha^{-1} to the top 20cm soil. Furthermore, at the harvest of cauliflower and leek roots from the respective crops with a CN ratio of 35 remained in the soil distributed over the soil root depth set to decompose: after cauliflower harvest 214 and 6.11 kg C and N ha^{-1} respectively remained in the soil while 255 and 7.28 kg C and N ha^{-1} respectively was set to decompose at leek harvest.

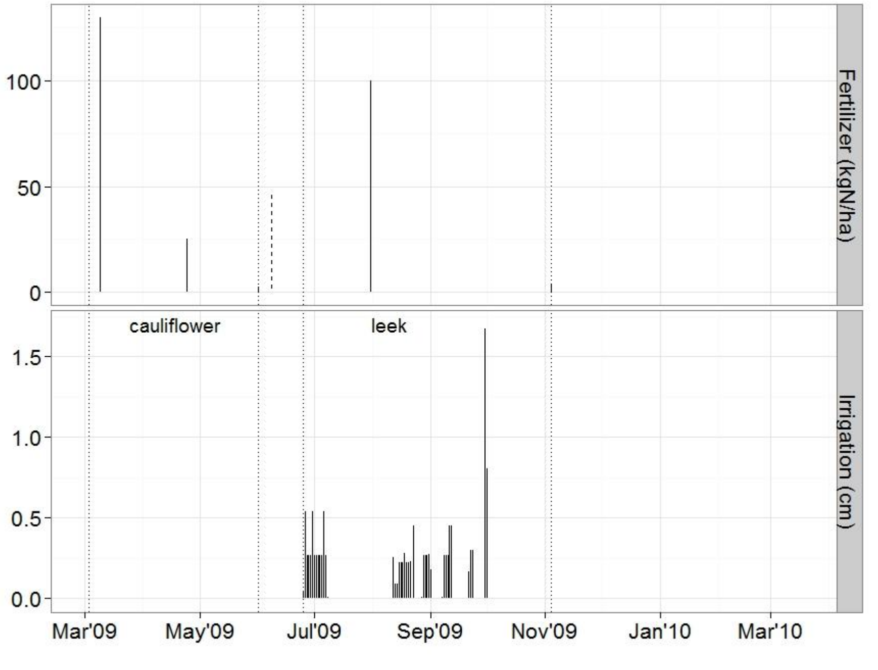

Figure 5-3 Overview of the fertilizer application and irrigation management during the crop rotation of cauliflower and leek in 2009 (dotted lines represent the start-end dates of the respective crops; in the upper graph the solid bars represent synthetic or inorganic fertilizer application and the dashed bars represent the organic fertilizer through root and crop residue incorporation at harvest and one week later respectively).

5.2 Model performance statistics

Both graphical techniques and quantitative statistics are recommended in model evaluation (Kersebaum et al., 2004; Legates and Mccabe, 1999). The visual inspection of the simulated and observed data is the most simple and straightforward approach to assess the model performance in terms of behaviour. Therefore, a first overview was given by the time series plot of the constituent of interest. In addition, the plot of observed versus simulated output was generated and complemented by a set of statistical indicators. Using only one statistic could be misleading as each of them provides information on a distinct aspect of the accuracy of the simulation and demonstrates various strong and weak aspects of the model. As recommended, the selection included at least one dimensionless statistic and one absolute error index with additional information such as the standard deviation of the measured data (Legates and Mccabe, 1999; Moriasi et al., 2007; Smith et al., 1997). The statistics are listed in Table 5-3 along with their calculation and their range with optimal value.

Table 5-3 Overview of statistics used in the model evaluation procedure (with observed (O_i) and simulated (S_i) values)

Statistic	Name	Equation	Perfect fit [range]
NSE	Nash-Sutcliffe modelling efficiency	$1-\frac{\sum_{i=1}^{n}(S_i-O_i)^2}{\sum_{i=1}^{n}(O_i-\bar{O})^2}$	1 $[-\infty\,;1]$
RSR	Root mean square error – observed standard deviation ratio	$\frac{\sqrt{\sum_{i=1}^{n}(S_i-O_i)^2}}{\sqrt{\sum_{i=1}^{n}(O_i-\bar{O})^2}}$	0 $[0\,;\,\infty]$
Pbias	percent bias	$\frac{100*\sum_{i=1}^{n}(S_i-O_i)}{\sum_{i=1}^{n}O_i}$	0 $[-100\,;100]$

Modelling efficiency or Nash-Sutcliffe efficiency (*NSE*)

The Nash-Sutcliffe efficiency (*NSE*) is a normalized statistic that determines the relative magnitude of the residual variance (“noise”) compared to the measured data variance (“information”) (Nash and Sutcliffe, 1970). NSE indicates how well the plot of observed versus simulated data fits the 1:1 line, i.e. how well the simulations correspond or coincide with the observations. This dimensionless statistic ranges between -∞ and 1, with 1 being the optimal value. Values lower than zero indicate that the mean observed value is a better predictor than the simulated value, which in turn implies a poor performance. NSE is similar to the commonly applied coefficient of determination (R^2) with the difference that it accounts for the predicted values from the simulation rather than from the fitted regression line. The latter would only quantify the linear association between observed and simulated data and might mask the true prediction accuracy.

Root mean square error (*RMSE*) – observations standard deviation (sd_O) ratio (*RSR*)

The commonly applied RSME expresses the overall deviation between observed and simulated data relative to the mean observed value, i.e. indicates the error in the unit of the constituent of interest. Based on the recommendation, it was standardized using the observations standard deviation (Moriasi et al., 2007; Singh et al., 2005). RSR incorporates the benefits of error index statistics and includes a scaling factor, so that the resulting statistic and reported values can be applied to various constituents. It varies from the optimal value of 0, indicating zero residual variation, to a large positive value. The lower RSR, the better the model simulation performance. If the RMSE is all or largely unsystematic, it is assumed that the model is as good as it can be (Willmott, 1981).

Percent bias (Pbias)

The bias in the total difference between measurements and simulations was determined by calculating the relative error (Addiscott and Whitmore, 1987). Expressed as a percentage, it is a measure for the average tendency of the simulated values to be consistently larger or smaller than the measured data. The optimal value of Pbias is 0, while positive and negative values indicate model under- and overestimation bias respectively.

5.2.1 Performance rating

Ultimate performance rating was achieved based on Moriasi et al. (2007) and Singh et al. (2004) recommendations which indicate the model prediction from poorly to (very) good as shown in Table 5-4. These ratings can be considered quite strict as data showed large variability and a daily time step was applied.

Table 5-4 Model performance ratings for the considered statistics

Model performance	NSE	RSR	Pbias (%)
Very good	$0.75 < NSE \leq 1.00$	$0.0 \leq RSR \leq 0.5$	$Pbias \leq 10$
Good	$0.65 < NSE \leq 0.75$	$0.5 < RSR \leq 0.6$	$10 < Pbias \leq 15$
Satisfactory	$0.50 < NSE \leq 0.65$	$0.6 < RSR \leq 0.7$	$15 < Pbias \leq 25$
Poorly	$NSE \leq 0.50$	$RSR > 0.7$	$Pbias > 25$

5.3 Calibration

The model output relates to four main state variables concerning (1) the crop biomass including its nitrogen content, (2) the soil water content, (3) the soil temperature and (4) the soil nitrogen content. Matching their simulation with the observed data led to the parameter values listed in Table 5-5, with data from literature and through calibration on the experimental data. Once the observed main variables were simulated as accurate as possible, the unobserved processes which they interact with, were assumed to occur as predicted given the selected parameter set. The output is evaluated in the following sections.

Table 5-5 Overview of the parameters of the integrated model: the value is specified if different for cauliflower/leek/fallow; references are provided from which the values are based on.

Parameter	Value	Unit (per day)
Crop growth (Dayan et al., 1993; Jones et al., 1989; Zekki et al., 1999)		
X_K	0.45/0.44/na	-
X_M	0.091	-
Q_e	0.0645	µmol CO_2 / mol photon
τ	0.0693	m / s
GREF	0.7	g(DM) / g(CH_2O)
Q_{10}	1.3/1.4	-
T_{ref}	20	°C
RMR_l	0.015/0.01/na	g(CH_2O) / g(DM)
RMR_f	0.015/0.007/na	g(CH_2O) / g(DM)
Rf_{sh}	0.09	-
RD_{ini}	5/17/na	cm
RD_{max}	70/60/na	cm
r_{di}	6.08e-7	cm / (°C day)
r_{le}	4.32e-4	cm / (°C day)
Runoff (Neitsch et al., 2011; USDA-NRCS, 1986; Woodward et al., 2003)		
CN_{ii}	79	-
C_{Ia}	0.05	-
slp	0	-
Evapotranspiration (Allen et al., 1998; DeJonge et al., 2012)		
c_1	900	-
c_2	0.34	-
alb	0.23	-
$K_{c,lai}$	0.8/0.5/na	-
f_K	2/2/4	-
$K_{c,max}$	1.1/1.2/1.1	-
KEP	0.463	-
Ztop	30	cm

Table 5-5 (Continued) Overview of the parameters of the integrated model: the value is specified if different for cauliflower/leek/fallow; references are provided from which the values are based on.

Parameter	Value	Unit (per day)
C:N flux (Bessou et al., 2013b; Jenkinson and Coleman, 2008; Li et al., 2006; Shaffer et al., 2001a; Smith et al., 2010)		
AmMin	0.5	mg N / kg
NiMin	0.1	mg N / kg
adsf	0.4905	-
biof	0.05	-
dfs	-0.06	-
$C{:}N_j$	40; 100; 8; 9.5 (dpm/rpm/bio/hum)	-
k_j	20; 0.3; 1.3; 0.02 (/365) (dpm/rpm/bio/hum)	/day
(*B:BH*)	0.46	-
PNR	1.74	mg N / kg
K_{nh4}	24	mg N / L
c	0.0016	-
a	0.0025	-
PDR	0.327	mg N / kg
K_{no3}	215	mg N / L
r	0.63	-
k_V	0.005	/day
Uptake (Jones and Kiniry, 1986)		
SRL	18000/16000	cm (root) / g
swcon1	0.00132	-
swcon3	7.01	-
$RTWU_m$	0.04	cm³ / cm(root)
$RTNH_{4m}$	0.0016	mg(N) / cm(root)
$RTNO_{3m}$	0.0016	mg(N) / cm(root)
aaf	0.16	-

5.3.1 Crop biomass and nitrogen demand

The gross photosynthesis, which accords to Acock's model (Acock et al., 1978) involves parameters assumed to be accurate and commonly used. Therefore, these parameters were kept unchanged and not subjected to the sensitivity analysis. On the other hand for maintenance respiration, the parameters regarding temperature effect (Q_{10}) and the maintenance coefficients (RMR_l and RMR_f) estimated at a reference temperature (T_{ref}) were fine-tuned to reach the observed potential growth.

In order to match the simulations with the observations, tabulated functions based on the latter were implemented for each crop specifically regarding fractioning of biomass into growing organs, specific leaf area, share of dead leaf in case of cauliflower and critical N content in the organs, all as a function of the observed accumulated thermal time and calculated developmental stage.

When the DVS changes, different fractions of daily acquired biomass will be distributed to the plant organs as shown in Figure 5-4. A constant root fraction of 9% of the shoot biomass is assumed.

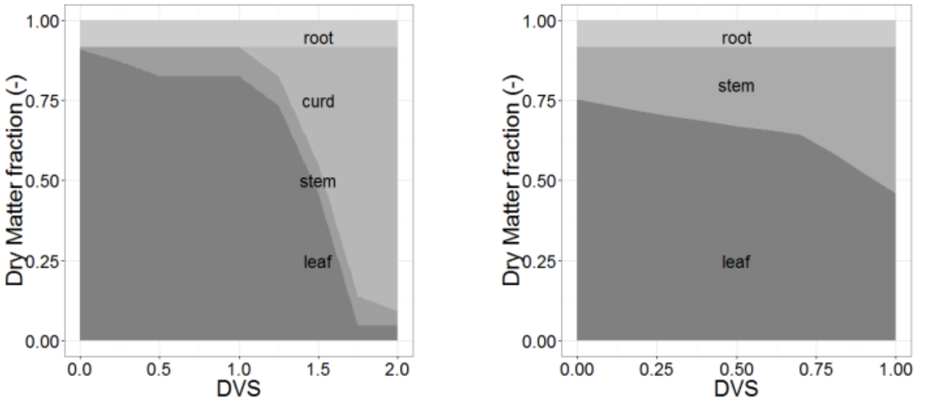

Figure 5-4 Compartmentation of daily produced dry matter as a function of the crop developmental stage (left for cauliflower, right for leek).

In case of cauliflower, the leaf dry matter increment is adjusted for leaf senescence as a function of the effective air temperature (Figure 5-5, left) once a DVS of 1.2 is reached. As the remaining green leaves grow, the LAI is estimated relating the leaf dry matter with the leaf area expansion through the specific leaf area (*SLA*), the latter being shown in Figure 5-6 (right). For cauliflower, the proportion of leaves expanding exponentially in the early life stage is much larger than later in the growing season. For leek, a different pattern is shown: as the stem thickens during the exponential growth, larger leafs are produced.

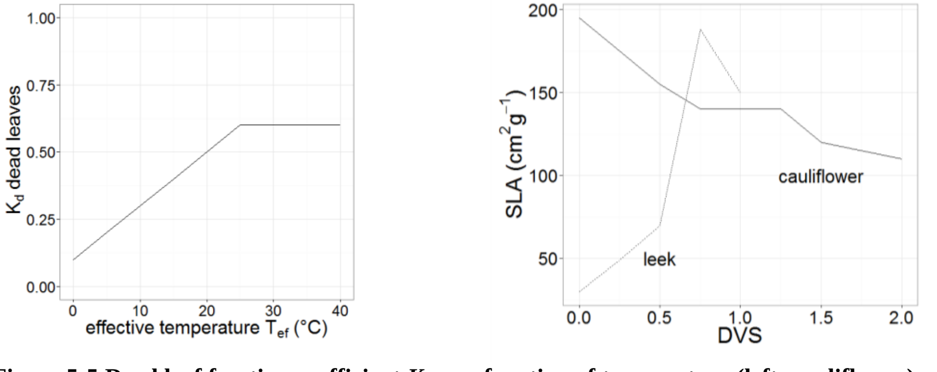

Figure 5-5 Dead leaf fraction coefficient K_d as a function of temperature (left; cauliflower) and specific leaf area (SLA) for cauliflower and leek leaves as a function of DVS (right).

Next, to support the plant organs growth, nitrogen has to be taken up. The N demand is related to the crops growth stage or DVS which suggest that a specific N concentration has to be realised to achieve optimal growth at a certain stage. The daily crop N demand is estimated along with the critical N concentration for the different plant organs (Figure 5-6). The additional N uptake per unit additional biomass, given a sufficient supply, declines as the crop grows.

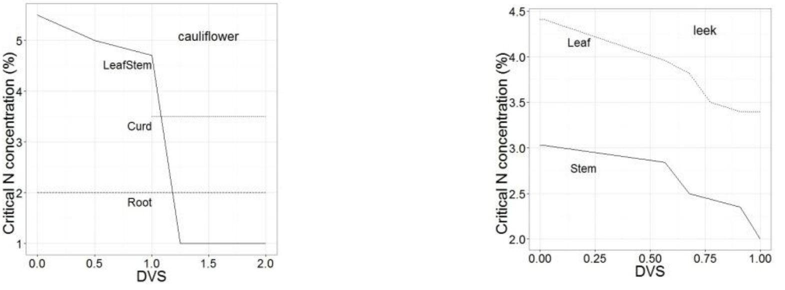

Figure 5-6 Nitrogen content in the plant organs of cauliflower (left) and leek (right) respectively in function DVS.

After incorporation of the crop modules within the main model also the maximum rooting depth (RD_{max}) was assessed as it influences the water and nitrogen uptake from the soil layers according to the root distribution.

Figure 5-7 shows the growth rotation cycle of cauliflower and leek for the calibrated year of 2009. The boxplots represent the observed biomass production at each of the destructive sampling days with an average harvest for cauliflower and leek of 188.1 (±42.6) g DM plant^{-1} and 60.9 (±17.3) g DM plant^{-1} or 7.5 and 11.0 t DM ha^{-1} respectively. The simulated values at harvest reached these observations quite well with values of 187.9 and 60.0 g DM plant^{-1} or 7.5 and 10.9 t DM ha^{-1}.
The predictions of the respective plant organs represented by the fruit and leaves were estimated closely to the observations. For cauliflower, the observed fruit and leaves made up to 28.5% and 71.5% of the shoot biomass versus 29.2% and 70.7% according to the simulated growth. The latter predicted for leek a share of 32.8% and 67.3% fruit and leaves respectively of the shoot biomass at harvest when observations showed ratios of 32.3% and 67.6% accordingly.
Simulations were considered (very) good based on visual interpretation and quantitative measures in accordance with the thresholds. Moreover, the performance statistics presented in Table 5-6, were calculated over the whole growing period and not limited to the moment of harvest. NSE and RSR values of 0.8-0.81 and 0.43-0.44 were reached respectively above and below the thresholds for the model performance to be considered as very good. Pbias values of 4.15, 7.66 and 2.24%, below the 10% threshold, for the respective shoot, fruit and leaf

dry matter confirmed a very good prediction of the dry matter in all the plant organs.

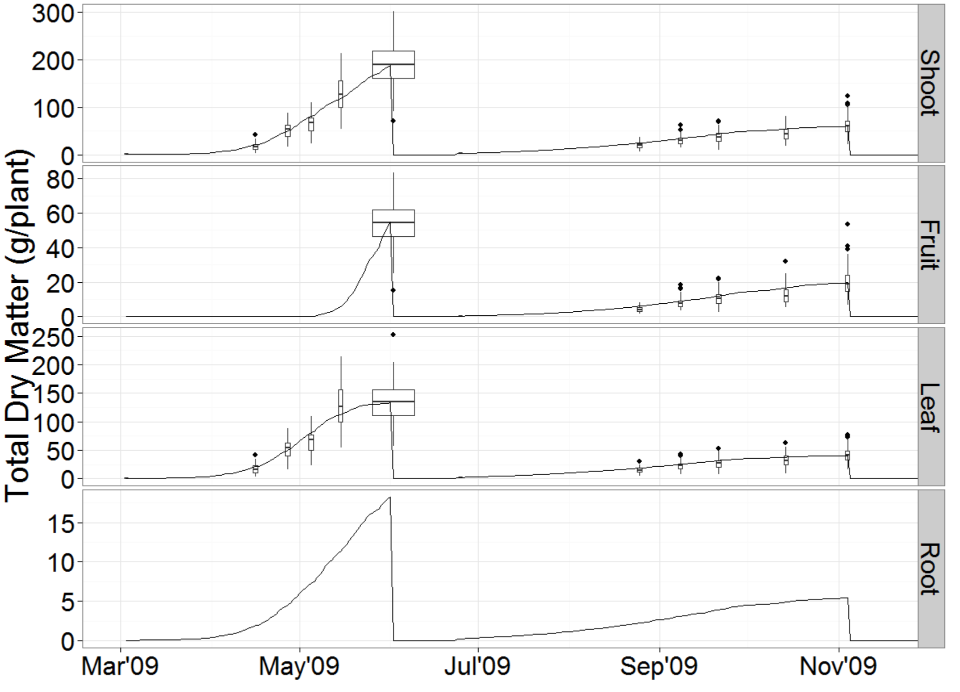

Figure 5-7 Calibration output of the biomass or dry matter for cauliflower and leek, i.e. for the shoot, the fruit, the leaves (including the stem for cauliflower) and the roots. Boxplots denote the measurements (the box shows the 1st and 3rd quartile around the median, whiskers are extended to values within the 1.5*box length or 1.5*interquartile range; outliers are shown by black dots) and simulated growth is presented by the solid line.

Commercially the biomass production is decisive for growers, yet it is the nitrogen content of the plant in its organs that is crucial as a minimum level has to be taken up to reach that daily potential biomass growth. Furthermore, nitrogen taken up by the plant cannot contribute to the environmental burden emitted to the air or leached with the percolation water, except for a potential share in the root biomass that remains in the soil and in the crop residues that are being incorporated into the soil. As Figure 5-8 shows and the results in Table 5-6 confirm, also the simulation of nitrogen uptake throughout the whole growing period matches the observations. At harvest, cumulative values of 6.4 and 1.6 gN plant^{-1} or 256 and 290.9 kgN ha^{-1} were predicted for cauliflower and leek when observations reached 6.8 (±1.4) and 1.7 (±0.5) gN plant^{-1} respectively.

The simulated N content in the respective plant organs were 29.7 and 70.3% of the shoot N content regarding the fruit and leaves of cauliflower respectively. The observations showed ratios of 30.9 and 69.1%. For leek, the simulated shares of N in the fruit and leaves were 25 and 75% respectively to the shoot as 23.5 and

76.5% were observed at harvest. Simulations of the crop N content were considered well to very good as well as the performance statistics in Table 5-6 indicate: NSE values that exceed the 0.65 threshold, RSR values which remain under 0.6 and Pbias values that not cross 10%.

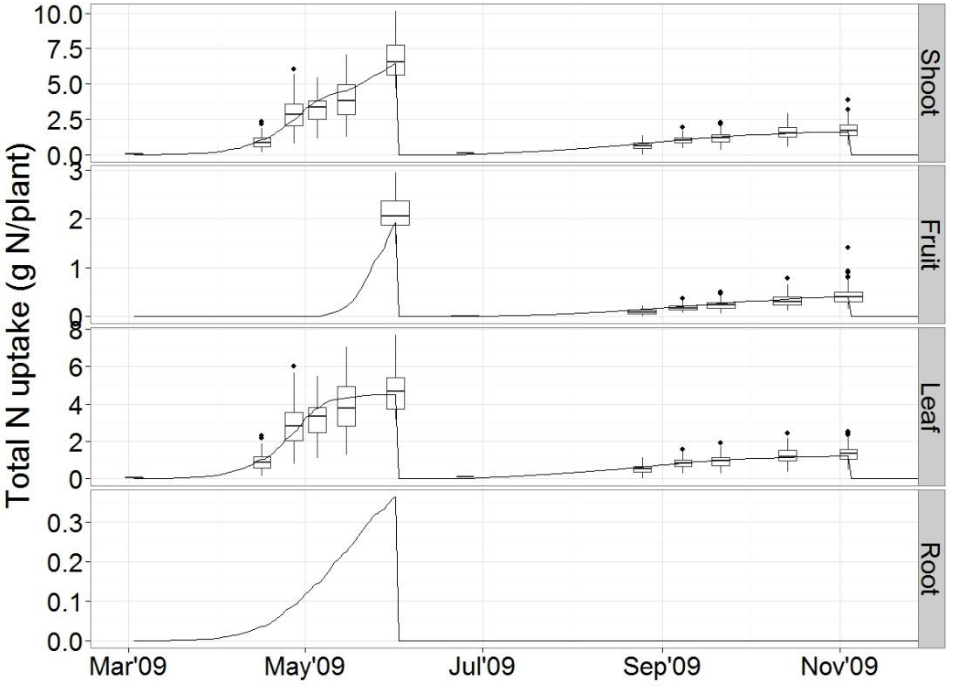

Figure 5-8 Calibration output of the total N demand for cauliflower and leek, i.e. for the shoot, the fruit, the leaves (including the stem for cauliflower) and the roots. Boxplots denote the measurements (the box shows the 1st and 3rd quartile around the median, whiskers are extended to values within the 1.5*box length or 1.5*interquartile range; outliers are shown by black dots) and simulated growth is presented by the solid line.

Besides the biomass and its nitrogen content, two extra properties of the leek crop are of interest: the diameter and length of the shaft. In the current crop model, their simulation was fitted on the observations during crop growth as a function of accumulated thermal time (see section 0). Simulated values of 3.6cm diameter and 19.1cm length approach the respective observations of 3.6 (±0.6) and 19.5 (±2.1) cm at harvest. Considering the whole growth period and shaft properties development, the statistics indicate a satisfying simulation regarding NSE and RSR values. Pbias values, well below 10%, even indicate good model performance regarding consistent data deviation.

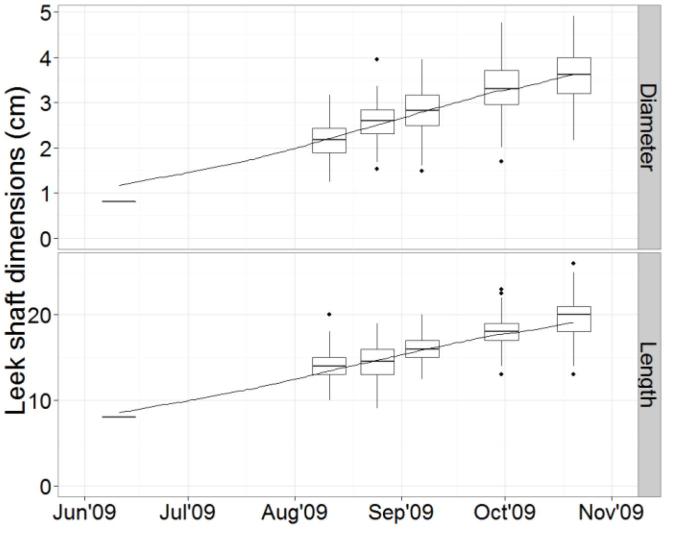

Figure 5-9 Calibration of the leeks shaft properties, i.e. the diameter and length. Boxplots denote the measurements (the box shows the 1st and 3rd quartile around the median, whiskers are extended to values within the 1.5*box length or 1.5*interquartile range; outliers are shown by black dots) and simulation is presented by the solid line.

Table 5-6 Overview of calibration output with model performance statistics (bold, regular and *(*) values indicate respectively a rating of poorly, satisfactory and (very) good).

		$\overline{O_i}$	sd_{O_i}	S_h	NSE	RSR	Pbias
Dry matter (g DM plant^{-1})							
Shoot	Cauliflower	188.1	42.6	187.9	0.83**	0.42**	5.73**
	Leek	60.9	17.3	60.0			
Fruit	Cauliflower	53.6	12.0	54.9	0.78**	0.47**	6.16**
	Leek	19.7	6.8	19.7			
Leaf	Cauliflower	134.6	34.8	132.9	0.80**	0.45**	4.77**
	Leek	41.2	11.5	40.4			
Root	Cauliflower	-	-	18.3	-	-	-
	Leek	-	-	5.4			
Nitrogen content (g N plant^{-1})							
Shoot	Cauliflower	6.8	1.4	6.4	0.72*	0.53*	2.98**
	Leek	1.7	0.5	1.6			
Fruit	Cauliflower	2.1	0.3	1.9	0.88**	0.35**	0.62**
	Leek	0.4	0.1	0.4			
Leaf	Cauliflower	4.7	1.2	4.5	0.72*	0.53*	2.14**
	Leek	1.3	0.4	1.2			
Root	Cauliflower	-	-	0.4	-	-	-
	Leek	-	-	-			
Leek shaft (cm)							
Diameter	Leek	3.6	0.6	3.6	0.56	0.66	-0.23**
Length	Leek	19.5	2.1	19.1	0.57	0.65	-1.97**

Additionally to the model performance statistics, the graphic representation in Figure 5-10 shows how well the data of observations versus simulations fit the 1:1 line.

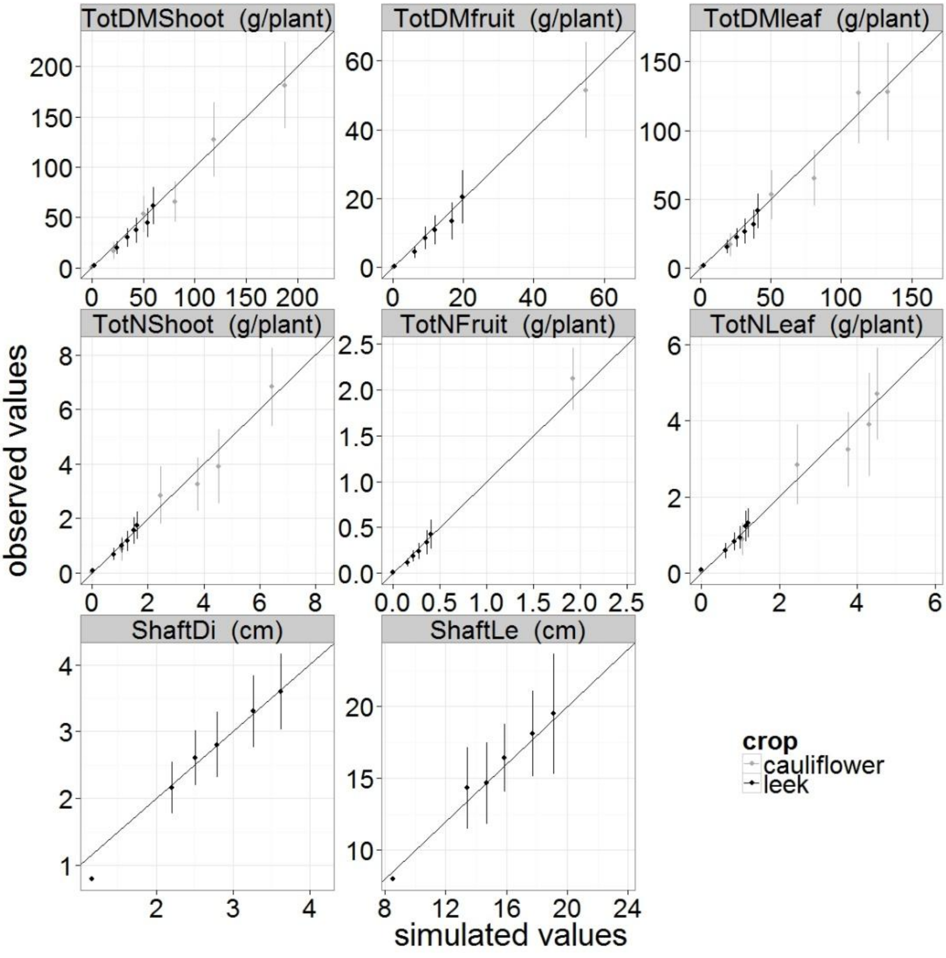

Figure 5-10 Overview of model performance observations versus simulation regarding crop dry matter (*TotDM*) and nitrogen content (*TotN***) for *shoot, fruit* and *leaf* for both cauliflower (grey) and leek (black); as well as stem or shaft properties, i.e. the diameter (*ShaftDi*) and length (*ShaftLe*) of the leek crop.**

5.3.2 Soil water

The soil water content was simulated and compared with the observations from the TDR sensors in two consecutive soil layers of 30 cm. As shown in Figure 5-11 the soil water content decreases during the crop growing periods marked by the vertical dashed lines. As the crop matures, water is taken up to meet the transpiration demands. The decrease in the lower soil layers is less pronounced due to lower root density. During summer, at the start of the leek cultivation and to compensate lack of precipitation, irrigation (bars) was applied. Yet, the simulated soil water content in the upper soil layer remained higher than the observed contents. Adjustment of soil water properties, water flow parameters and/or root characteristics did not close the gap between observed and simulated soil water in the upper layer. Additionally, attention had to be paid at calibration of crop growth and soil nitrogen content (see further) which all interact. Thus, it seems the model underestimates the soil water uptake, whether or not in combination with inaccurate irrigation data. The daily amount of irrigated water was not monitored very accurately due to the mechanism of the irrigation sprinkler and the estimation based on operation time and debit. A recalibration at the start of leek growth and a small but consistent adjustment of irrigation was applied considering the uncertainty in the observed data.

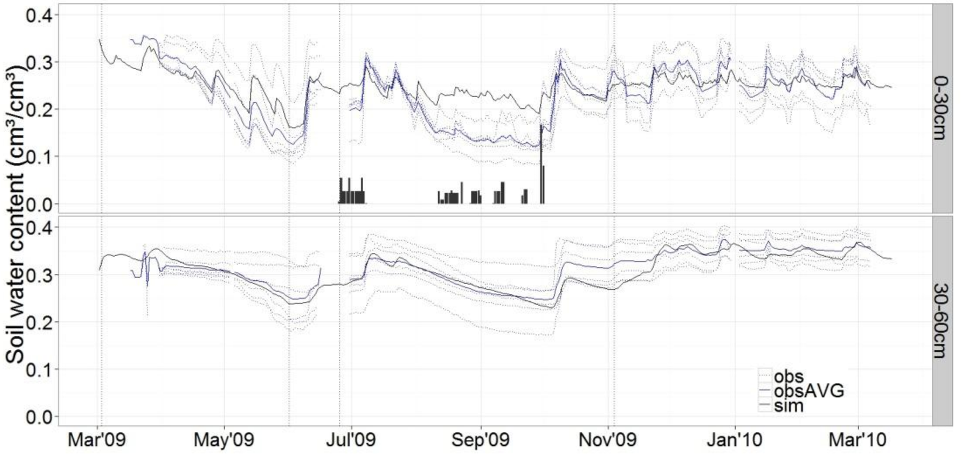

Figure 5-11 Calibration of soil water content in soil layers 0-30cm (upper) and 30-60cm (lower) with observations (*obs, dotted blue lines*), their average value (*obsAVG, solid blue line*) and the simulated values (*sim, solid black line*). Vertical dashed lines represent the growing periods of cauliflower and leek. Black bars indicate the irrigation scheme.

Ultimately, this resulted in a NSE and RSR value (see Table 5-7) that approached but did not reach the desired thresholds to be considered as a satisfying simulation. If the irrigation period was excluded from analysis, the model performance rating was good, as shown by the values in brackets. Regarding the lower layer and the Pbias for both, a very good model performance was achieved.

Table 5-7 Calibration of soil water content in two consecutive soil layers of 30cm with respective model performance statistics (values in between brackets indicate model performance excluding data from the irrigation period with high uncertainty; (bold, regular and *(*) values indicate respectively a rating of poorly, satisfactory and (very) good)).

	$\overline{O_i}$	sd_{O_i}	$\overline{S_i}$	NSE	RSR	Pbias
Soil water content (cm³ water*cm⁻³ soil)						
0-30cm	0.23	0.06	0.25	**0.48** (0.68*)	**0.72** (0.57*)	7.67** (2.06**)
30-60cm	0.31	0.04	0.31	0.82**	0.42**	0.02**

The graphical representation of the model performance regarding soil water content (SWC) is shown in Figure 5-12 where observed data was plotted against the simulated data to visualize how well these data would fit the 1:1 line.

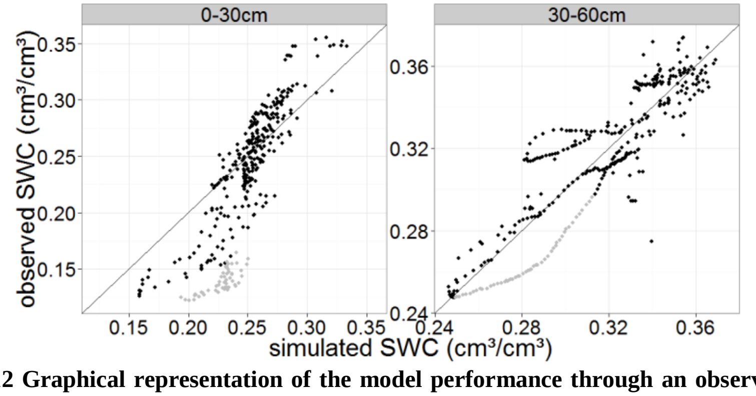

Figure 5-12 Graphical representation of the model performance through an observed versus simulated soil water content plot for the whole simulation period (data during irrigation period is shown in grey).

5.3.3 Soil temperature

As soil carbon and nutrient cycling is sensitive to temperature changes (see section 4.2) and the effect of climate change is gaining interest, the accurate prediction of soil temperature is an important model component (Zhang, 2010). Simulations and observations of the soil temperature at 15 and 45cm from the surface were compared. As commonly found, the measured soil temperatures correlated strongly with the air temperature and decreased with increasing depth. The model successfully simulated the overall temporal pattern for soil temperatures at both depths, as shown in Figure 5-13 and confirmed by the performance statistics presented in Table 5-8 and visualized in Figure 5-14. A small overestimation of soil temperature, especially when crops are mature, suggest the model does not take into account the effect of plant shading as mentioned by Sándor and Fodor (2012) and Liu et al. (2013). Also during winter when temperature drops towards zero degrees, the fluctuation of simulated soil temperatures was more pronounced than was observed. This period of recurrent days of frost seemed to freeze the soil water which releases energy and prevents the temperature from decreasing as far as the model predicts. This requires further refinement of the algorithm.

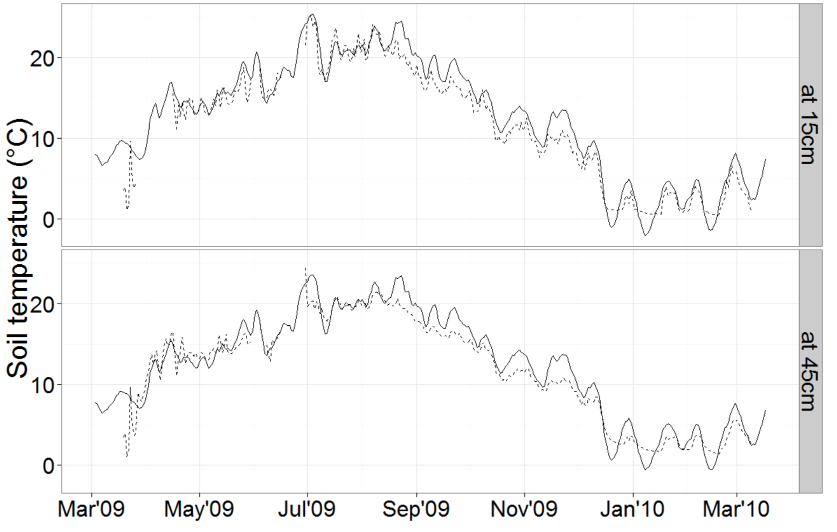

Figure 5-13 Calibration of soil temperature at 15 (upper) and 45cm depth (lower) with observations (dashed lines) and simulated values (solid lines).

Table 5-8 Calibration of soil temperature at two soil depths with respective model performance statistics (bold, regular and *(*) values indicate respectively a rating of poorly, satisfactory and (very) good)).

	$\overline{O_i}$	sd_{O_i}	$\overline{S_i}$	NSE	RSR	Pbias
Soil temperature (°C)						
At 15cm	11.44	7.19	12.53	0.93**	0.26**	9.59**
At 45cm	11.58	6.26	12.35	0.92**	0.28**	6.65**

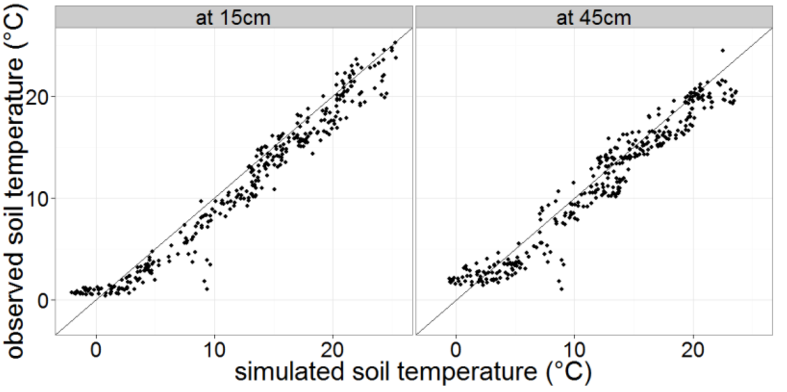

Figure 5-14 Graphical representation of the model performance through an observed versus simulated soil temperature plot for the whole simulation period.

5.3.4 Soil mineral nitrogen

In order to apply and control additional fertilizer efficiently, an estimation of the soil mineral nitrogen content is required. It was simulated and compared with the observations from the soil samples in two consecutive soil layers of 30 cm, similar to the soil water content. Despite a limited number of observations in time, the model approached the overall trend of the soil nitrogen content during the rotation cycle as shown in Figure 5-15. Yet, the irregular offset of the model from the observations over time suggest further adjustment is required regarding the N flows affecting the mineral N pool. The large amount of nitrate measured at the first quarter of leek cultivation questions mainly the steep decline at the end of cauliflower and/or the effect of root decay and crop residue incorporation. At the moment of assessment with the given process functions, adaptation of parameter values did not result in improvement. Multiple processes interacting on the ammonium N pool (adsorption, mineralisation/immobilisation, volatilisation, nitrification, drainage and uptake) with different rates, still lack of detailed knowledge and the limited amount of observations made this calibration extremely difficult.

Consequently this resulted in poor performance ratings as presented in Table 5-9 except for the nitrate which reached almost in both layers acceptable values for NSE and RSR. The Pbias for nitrate showed no consistent error.

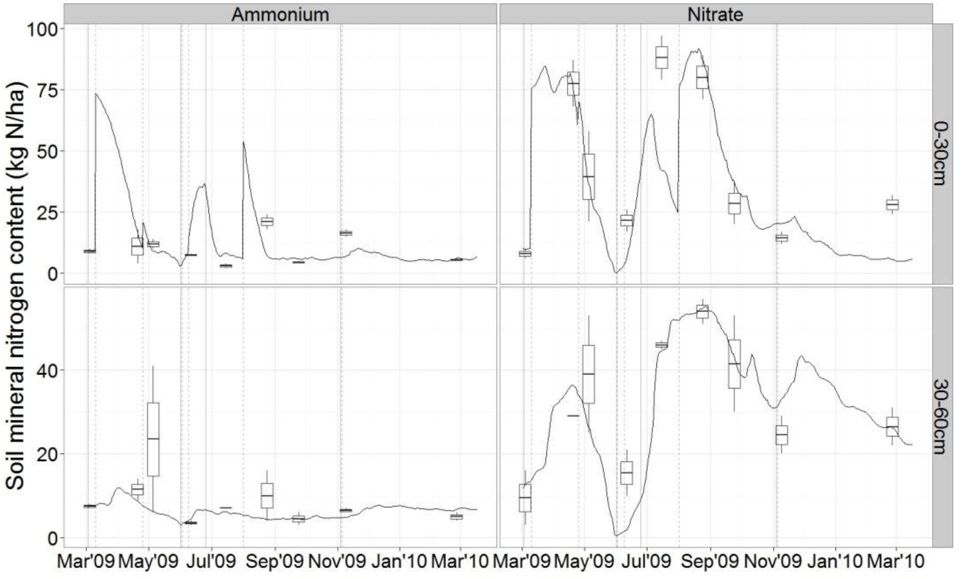

Figure 5-15 Calibration of the soil mineral nitrogen content as nitrate and ammonium (in kgN ha^{-1}) in soil layers 0-30cm (upper) and 30-60cm (lower) with observed values represented by respectively the boxplots (the box shows the 1st and 3rd quartile around the median, whiskers are extended to values within the 1.5*box length or 1.5*interquartile range; outliers are shown by black dots) and simulation shown by the solid line. Vertical lines represent the growing periods of cauliflower and leek.

Table 5-9 Calibration of soil mineral nitrogen content (for ammonium and nitrate separately) in two consecutive soil layers of 30cm with respective model performance statistics (bold, regular and *$^{(*)}$ values indicate respectively a rating of poorly, satisfactory and (very) good)).

	$\overline{O_i}$	sd_{O_i}	$\overline{S_i}$	NSE	RSR	Pbias
Soil ammonium content (kg N ha^{-1})						
0-30cm	10.0	6.3	10.07	**-0.75**	**1.32**	0.70**
30-60cm	8.8	8.7	6.0	**-0.08**	**1.04**	**-32.12**
Soil nitrate content (kg N ha^{-1})						
0-30cm	42.8	31.1	35.6	0.55	0.67	-16.80*
30-60cm	31.7	15.9	31.0	0.56	0.66	-2.13**

5.3.5 Other soil processes

Other processes were not measured and therefore could not be calibrated directly, although they still affected the output variables discussed so far. An overview of these processes and corresponding model output is given discussed here. As the simulation of the crop biomass, its nitrogen content, the soil water content, the soil temperature and the soil nitrogen content was considered accurate under given conditions, it is assumed the processes that had an indirect effect on these

outputs, were also well simulated. This included on the one hand the water flow related processes of interception, runoff, drain/deep percolation, soil evaporation, plant transpiration or water uptake and the net soil water content change. On the other hand the nitrogen flow related processes included the net soil nitrogen content change due to adsorption and mineralisation/immobilisation, and N emissions (ammonia volatilisation, (de)nitrification and leaching). The soil water and nitrogen flows are presented in Figure 5-16 to Figure 5-18.
An assessment was made whether the outputs were in line with the findings in literature, although it was not straightforward to compare with other case studies even if climate conditions, crop types or soil properties tended to be similar. Most of the time, wide ranges of process results were reported due to the large variability among the sites and conditions examined in the different studies.

Water flow

An overview of the quantitative soil water flows in the calibration period is listed through the balance in Table 5-10.
From the incoming 731mm of rain and additional 128.5mm of irrigated water (*Irrig*), almost 9% is intercepted by the crop (*Interc*), especially in the second half of cultivation as the crop cover increased. Ranges from 10-20% to 22-58% of rainfall were reported depending on rainfall intensity, vegetation type, structure and cover and potential evaporation (de Jong and Jetten, 2007b; Kozak et al., 2007). As earlier addressed, the intercepted water is evaporated prior to the plant transpiration or actual water uptake from the soil.
When the amount of throughfall exceeds the infiltration capacity of the soil, runoff may occur. During the moments of heavy rainfall, peaks of water runoff (*RO*) were simulated accumulating to 11% over the whole rotation cycle. Although no slope was visually and virtually present, high rainfall intensity in combination with soil properties could lead to surface runoff values reaching up to 17.9% of the rainfall (Batelaan and De Smedt, 2007; Park, 2012; Tarboton, 2003). The total amount of soil water in the soil profile (*SWCtot*, cm) slightly decreased by 6% after 381 days from the start of cauliflower, as most of the water left the ‘soil system’ through evapotranspiration by 58% or 498mm. As the crops matured, plant transpiration (PT_a) became more dominant over soil evaporation (SE_a), resulting in 60% of evapotranspiration at the end of the cycle. Global annual terrestrial evapotranspiration averagely ranges from 415-585 mm, dominated by 59% of transpiration (Wang-erlandsson, 2014). Meteorological data in Belgium report relative larger values of 450 up to 650 mm year^{-1} with an increasing trend over the last decade (Batelaan and De Smedt, 2007; Brouwers et al., 2015), with still daily values between 0.02 and 4.5mm day^{-1} (Sepulcre-Cantó et al., 2013). Given the lack of water stress, the actual water uptake meets the plant transpiration demand. As addressed earlier, calibrating the soil water content (see section 5.3.2), underestimation of the soil water uptake and therefore the potential plant transpiration requires further model analysis. Lowering the simulated interception, adjustment of the K_c crop coefficient and/or considering

an alteration or replacement of the Penman-Monteith evapotranspiration model should be looked into. Comparison of the simulated transpiration with the transpiration estimated using the transpiration efficiency according to Kemanian et al. (2005) confirms the underestimation. The ratio of above ground biomass to water transpiration, adjusted for a seasonal average vapour pressure deficit for each growth period, reached for cauliflower and leek respectively to 66% and 88% of the theoretical value of 5-6 gBM Pa g^{-1} water for a C3- crop. Yet, efficiency values remained within the range of values reported (Kemanian et al., 2005).

Furthermore, soil water percolated deeply out of reach for plant uptake at the early stage of cauliflower cultivation (14.1%) and during the fallow period over winter (85.9%). These periods showed correspondingly high water content levels due to higher rainfall, no uptake by the crop and limited soil evaporation. This deep percolation (*Perc*) into the groundwater table mounted up to 203mm, or 24% of the soil water including the supplements of rain and irrigation. Related literature reports leaching values of 161 to 369 mm $year^{-1}$ (Beaudoin et al., 2005).

Table 5-10 Simulated soil water balance for the calibration period.

Water flow	(cm)
Rain	+73.13
Irrigation	+12.85
Interception	-7.62
Runoff	-10.06
Net SWC_{tot} change	+1.84
Soil evaporation	-20.02
Plant transpiration = water uptake	-29.79
Deep percolation	-20.33
Balance	≈0

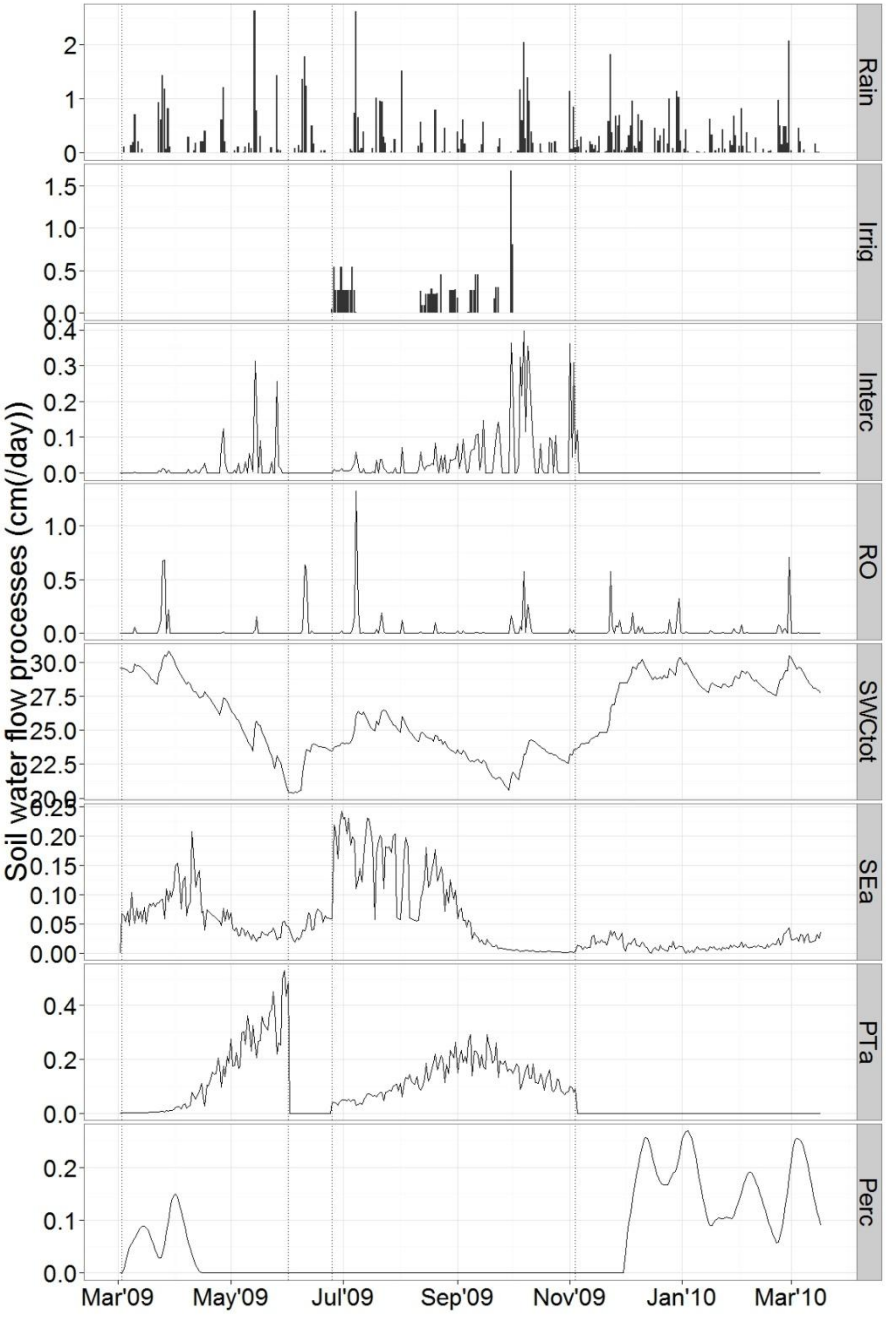

Figure 5-16 Overview of the simulated daily soil water flow processes (cm day^{-1}), i.e. rain, irrigation (*Irrig*), interception (*Interc*), surface runoff (*RO*), actual soil evaporation (*SEa*), actual plant transpiration (*PTa*) and deep percolation (*Perc*), during the calibration year 2009, affecting the total soil water content over 90 cm depth (*SWCtot, cm*).

Nitrogen flow

An overview of the quantitative soil nitrogen flows in the calibration period is listed through the balance in Table 5-11.

As inorganic and organic nitrogen fertilizer (*fert*) is added inorganically through broadcast application on the surface of the soil (255 kg N ha^{-1}) or organically through incorporation of crop residue or decaying roots after harvest (105.2 kg N ha^{-1}), the soil N pools are affected. The soil organic matter pools (*N*) mineralized 4.15 kg N ha^{-1} in January up to 104.7 kg N ha^{-1} in June which flats out to a daily average of 1 kg N ha^{-1} day^{-1} over the whole cycle. Peaks in SOM-N are due to crop residue being incorporated in the top 30cm soil. Mineralisation (*MI*) added up to 395.1 kg N ha^{-1} or 3.2% of the initial soil organic matter N content, without any day of net immobilisation going backwards. The model predicted immobilisation from the resistant plant material (RPM) pool after harvest due to root decay, which is however compensated by higher decomposition of the other three organic matter pools (DPM, BIO and HUM). Monitoring gross mineralisation or immobilisation is rather difficult. Consequently net mineralisation in literature showed large differences in cumulative values from 98 to 508 kgN ha^{-1} according to different models (Kersebaum et al., 2004). The relative high mineralisation rate might be caused by the history of the experimental parcel which was characterised by high organic fertilisation with large amounts of organic nitrogen. Running the model with decreased decomposition rates, significantly underestimated the mineral nitrogen contents in the soil layers.

Three applications of mineral N fertilizer resulted in peaks of both the ammonium pool (NH_4) and the nitrate pool (NO_3), the former being in equilibrium with the ammonium adsorbed on the clay minerals (*ADS*). With increasing ammonium content, nitrification (*NIT*) raised the nitrate content with 435.3 kg N ha^{-1}, while only a limited amount of 0.81 kg N ha^{-1} denitrified (*DENIT*).

Most nitrogen is taken up (*UPT*) by the crops, with 76% and 92% as nitrate by cauliflower and leek respectively. Overall, the soil nitrogen content decreased with 269.9 kg N ha^{-1} or 2.2% over the rotation cycle. While soil organic matter N and ammonium, adsorbed as well as free, decreased by 2.4 and 24.4% respectively, the nitrate content increased by 71.1%.

Along with these processes nitrogen is also emitted to the air and groundwater which in turn burdens the environment as it contributes to climate change, acidification and eutrophication in terms of impact categories commonly investigated with life cycle assessments (cf. Chapter 3).

Related to the mineral N fertilizer applications, a share of the ammonium is volatilized as ammonia (*VOL*) which added up to 2.3 kg N ha^{-1} for the whole cycle, which would be 1% of the inorganic fertilizer added. The empirical approach reports 2% of ammonium nitrate that is lost as ammonia, while Misselbrook et al. (2004) estimates a 1.1% loss of ammonia from ammonium nitrate application on national scale.

During nitrification the intermediate by-products nitrogen oxide (*NO_x*) and dinitrogen oxide (*N_2O*) were emitted with cumulative amounts of 1.1 and 1.2 kg N ha^{-1} respectively, which comprises only 0.53% of the amount nitrified into nitrate. Under denitrifying conditions nitrate is ultimately converted to the harmless end product N_2 for 75.7%, while 24.3% or 0.2 kg N ha^{-1} is emitted as N_2O. Different models on common datasets from Germany also showed a minor role by denitrification and subsequently small amounts of N_2O losses (Kersebaum et al., 2004). Data from field studies from the peer reviewed literature was summarized by Bouwman et al. (2002a) to assess main factors regulating nitrogen oxide losses. Depending of N application rate, with soil organic carbon content between 1% and 3%, a coarse soil texture class and other factor classes matched with current experimental data, mean values would reach from 1.1 to 6.8 kg N_2O-N ha^{-1} , which corresponds with reported values in Regina et al. (2013) of 0.3-5.4 kg NO-N ha^{-1}. Although N_2O generally would dominate NO_x in gas emissions, it is less apparent in coarse textured and well-drained soils.

In the deeper soil layers, nitrogen (most as nitrate, very little as ammonium) percolates (*Nleach*) along with the drained water which resulted in 4.4 and 56.1 kg N ha^{-1} lost from the soil at the early stage of cauliflower cultivation and the fallow period after leek harvest respectively. Corresponding with the amount of water leached, average concentrations of nitrogen were 15.3 and 32.2 mg N L^{-1} in the respective periods. The latter equals to 142.6 mg NO_3^- L^{-1} which would by far exceed the European threshold of 50 mg NO_3^- L^{-1} (see introductory chapter section 1.2.2). Related literature reported yearly nitrogen leaching from 10-83 kg N ha^{-1} (Beaudoin et al., 2005; Li et al., 2006) up to (simulated) 189 kg N ha^{-1} that can be lost from the bottom of the rooted soil zone at 90 cm (Kersebaum et al., 2004). Loamy soils showed lower leaching compared to sandy with concentrations around 31 mg L^{-1}.

Table 5-11 Simulated soil nitrogen balance for the calibration period.

N flow	(kgN ha^{-1})
Organic fertilizer	+105.21
Mineral fertilizer	+255.0
Net N_{org} change	+289.87
Net N_{min} change	-20.02
N uptake	-564.15
NH_3 volatilisation	-2.29
NO_x (nitrif)	-1.09
N_2O ((de)nitrif)	-1.42
N_2	-0.62
N Leaching	-60.49
Balance	≈0

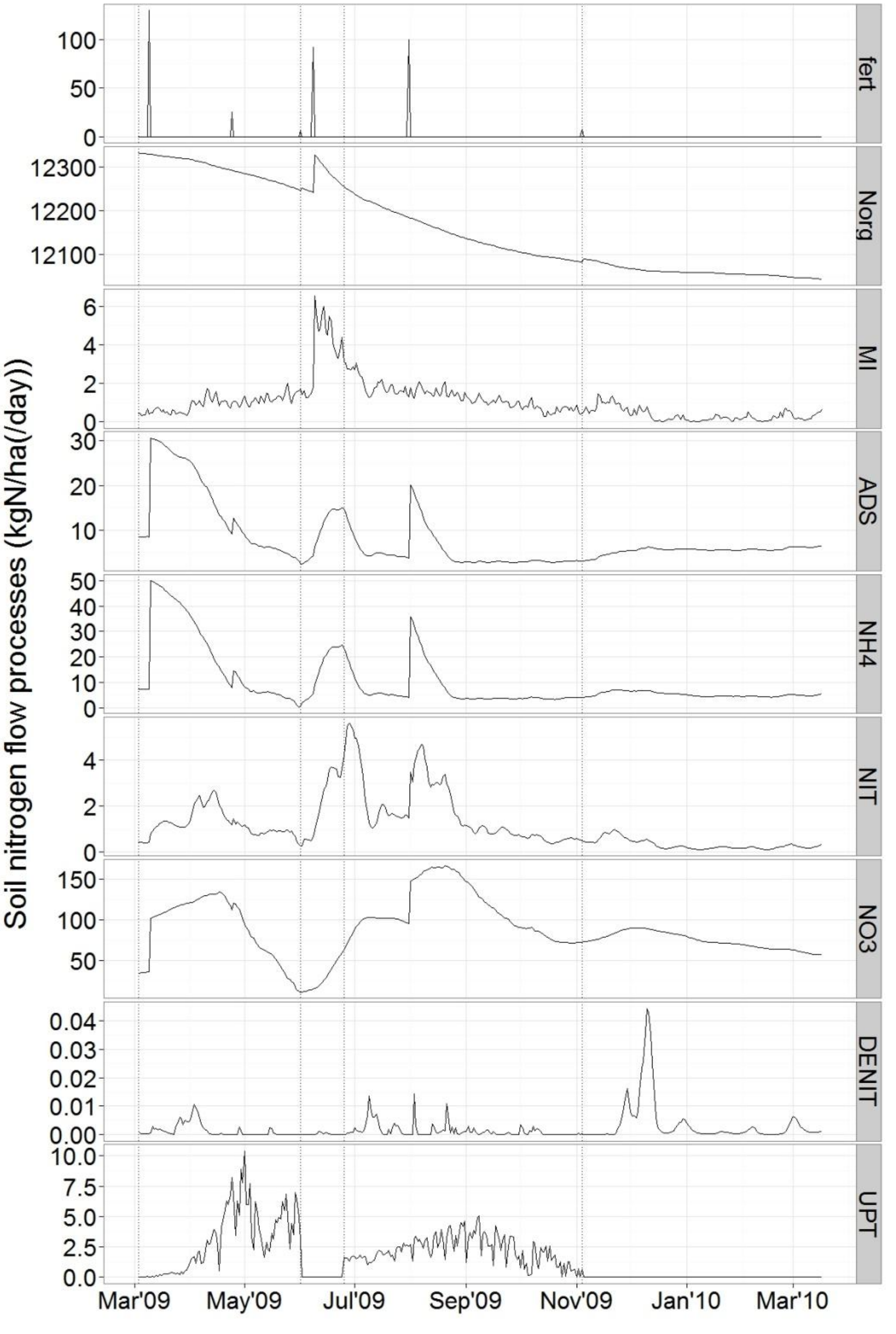

Figure 5-17 Overview of the simulated daily soil nitrogen flow processes (kgN ha^{-1} day^{-1}), i.e. fertilizer application (*fert*), mineralisation (*MI*), nitrification (*NIT*), denitrification (*DENIT*) and soil nitrogen uptake by crops (*UPT*), during the calibration year 2009, affecting the total soil nitrogen contents (kgN ha^{-1}) of soil organic nitrogen (N_{org}), free (NH_4) and adsorbed (*ADS*) ammonium and nitrate (NO_3).

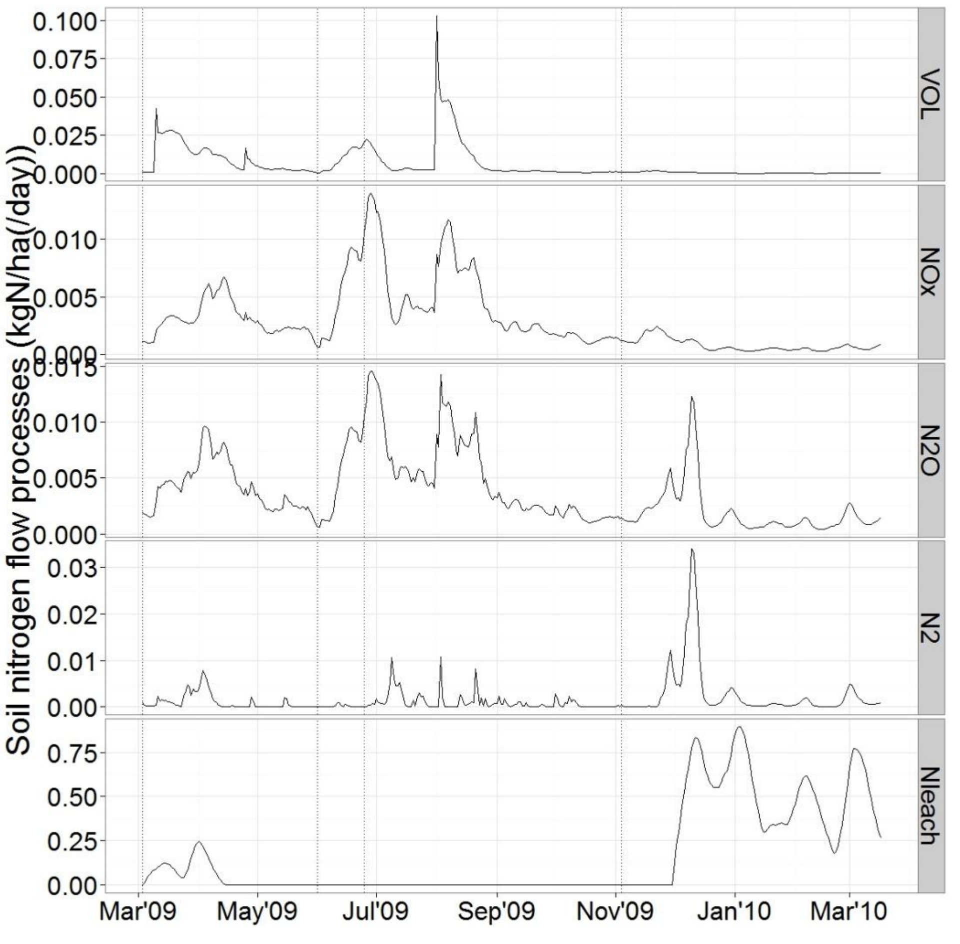

Figure 5-18 Overview of the simulated daily soil nitrogen emissions (kgN ha^{-1} day^{-1}) affecting the soil mineral nitrogen content during the calibration year 2009: ammonia volatilisation (*VOL*), nitrogen oxide (*NO_x*), dinitrogen oxide (*N_2O*), dinitrogen (*N_2*) and nitrogen leaching (*Nleach*).

5.4 Sensitivity

On the one hand a sensitivity analysis allowed an estimation of the key parameters for calibration purposes in order to match the simulation with the observations as assessed above. On the other hand these parameters were validated as well by a local sensitivity analysis that considered fixed perturbations around the local estimates of the calibrated model parameters (see Table 5-5). The model response was assessed for a fixed change in parameter values, i.c. 10% lower and higher. The sensitivity of the output variables to the model parameters and input factors will be defined as the variation caused on the output variable per unitary variation on the model parameter or input factor according to Cooman (2002). Quantification is assessed with the coefficient of variation (*CV*, %):

$$CV_t = \frac{sd_t}{mean_t} * 100 \tag{127}$$

Where CV_t is the coefficient of variation (%) of the model response variable at time *t* with the respective standard deviation sd_t and mean $mean_t$.

The ratio of the CV of a model output to the CV of the parameter or input factor, i.c. 10%, provides a unit less measure of sensitivity (*S*). It furthermore considers the model output variable to be insensitive or sensitive to the model parameter or input factor if variation of the latter causes a respectively smaller or larger variation on the output.

$$S_t = \frac{CV_t}{10\%} \tag{128}$$

Where S_t is the sensitivity of a model output variable at time *t* to fixed change of the parameter or input factor value, i.c. 10%;
CV_t is the coefficient of variation (%) of the model response at time *t*.

The results from the sensitivity analysis are shown in Figure 5-19 and Figure 5-20 and listed in Table 5-12. Numbers 1 to 3 of indexed parameters refer to the three consecutive soil layers of 30cm (0-30cm; 30-60cm and 60-90cm). Results are limited on the one hand to the parameters that are influential according to the CV ratio (S_t) and on the other hand to the cumulative model response variables that are sensitive to those parameters and directly affect LCA results. Also, two runs of the parameter set were excluded from analysis as the increase of the bulk densities of the two lower soil layers without lowering saturation limits would create unrealistic responses regarding moisture effect on the denitrification process. Due to the relation between bulk density, total porosity and saturation, high water content would exceed the potential water filled pore space that affect N emissions during (de)nitrification. Furthermore, as sensitivity might change over time, three S_t values were calculated (separated by a dash): at the harvest time of each crop and at the end of the simulation period.

Crop growth

Sensitivity analysis showed no effect of changing any of the parameters in Table 5-5 neither on the crop growth, on the dry matter nor on the nitrogen uptake. No change of any parameter caused any occurrence of water or nitrogen stress. A maximum CV of 4.7% was achieved on the N uptake by the cauliflower crop by changing the bulk density of the top 30cm soil layer.

Soil water and nitrogen flows

Looking into the water flow processes, interception was not affected as no effect on crop growth was detected. Runoff (*RO*) on the other hand was found to be sensitive to the soil water characteristics of bulk density, field capacity and saturation limit of the top layer and to two parameters of its simulation function: the regression coefficient (C_{Ia}) and especially the curve number for average moisture content (CN_{II}). The latter, along with the soil water characteristics as well, seemed to have considerable effect on the deep water percolation (*Perc*) and the nitrogen that is transported with it (*Nleach*). The results of nitrogen leaching were similar for its constituents ammonium and nitrate. Considering these parameters and input factors, it is the field capacity of the top layer that resulted in a bigger variation of the percolation and N leaching than 10%. Furthermore, K_{cml}, the maximum K_c factor for evapotranspiration during leek cultivation at wet soils had a small effect on water percolation at the end of the simulation period. Other parameters that were influential to the N leaching were the N flow process related parameters: i) *biof*, $C{:}N_{BIO}$ and k_{BIO} (only at the end of simulation) representing the share of the BIO pool of the total soil organic matter, its C-N ratio and decay rate, ii) *dfs*, a depth factor on decomposition, iii) *adsf*, an adsorption coefficient (only on NH_4 leaching, at all times) and iv) *PNR*, the potential nitrification rate (only on NH_4 leaching at the end of simulation).

Nitrogen air emissions

Volatilisation of ammonia (NH_3) and nitrous oxide (N_2O) from the top layer were sensitive to the top layer's field capacity, regarding cumulative values over time till cauliflower harvest. Nitric oxide (NO_x) emissions from the two lower soil layers on their turn showed at each time of interest a bigger variation effect on the output due to variation on the *dfs* factor which affects decomposition and the following nitrification of mobilized ammonium. The most sensitive model responses however were the N_2O emissions from the two lowest soil layers. Especially below 60cm in the soil, the response was sensitive at each time to the lowest layers' bulk density (only with -10%) and the field capacity of the upper layer as well. Also the change in the maximum K_c factor for cauliflower and leek at wet soil conditions created ultimately at the end of the simulation a bigger variation on the cumulative N_2O release than 10%.

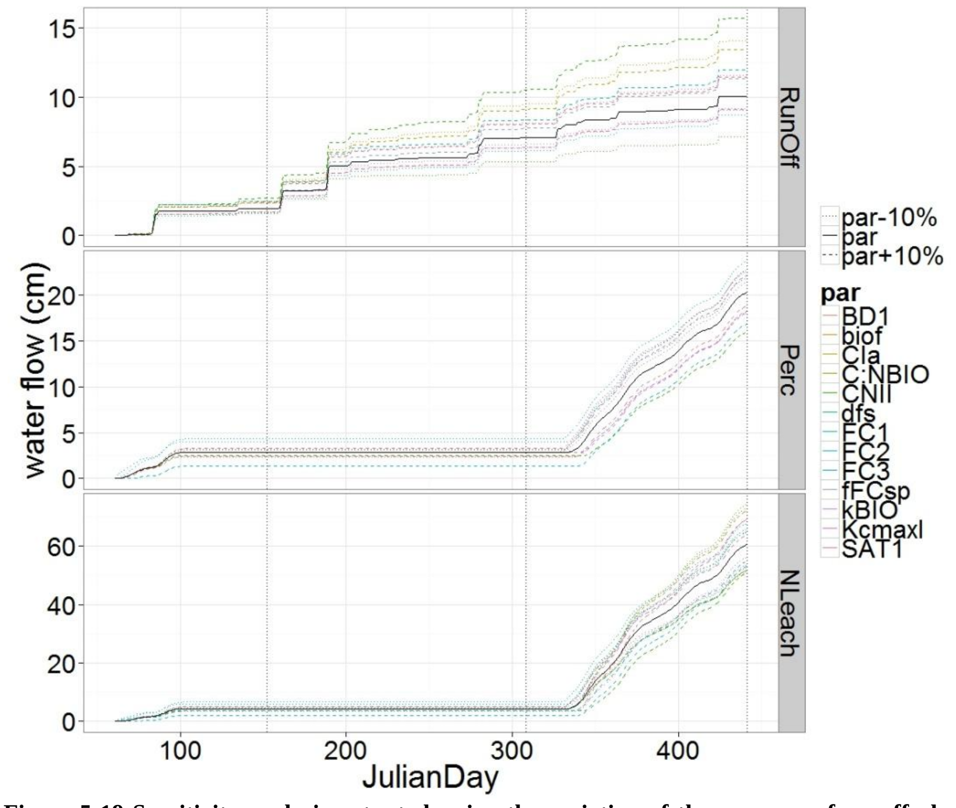

Figure 5-19 Sensitivity analysis output showing the variation of the response of runoff, deep water percolation (*Perc*) and nitrogen leaching (*Nleach*) to a 10% variation of the following parameters: bulk density of top layer (*BD1*), field capacity in all three layers (*FC1*, *FC2*, *FC3*), saturation limit of top layer (*SAT1*), BIO pool fraction of SOM (*biof*), C-N ratio of BIO pool ($C{:}N_{BIO}$), decay rate of BIO pool (k_{BIO}), depth factor for decomposition (*dfs*), initial abstraction coefficient for runoff (C_{Ia}), curve number for average moisture content (CN_{II}) and maximum crop Kc factor for wet soils during leek cultivation regarding evapotranspiration (K_{Cmaxl}).

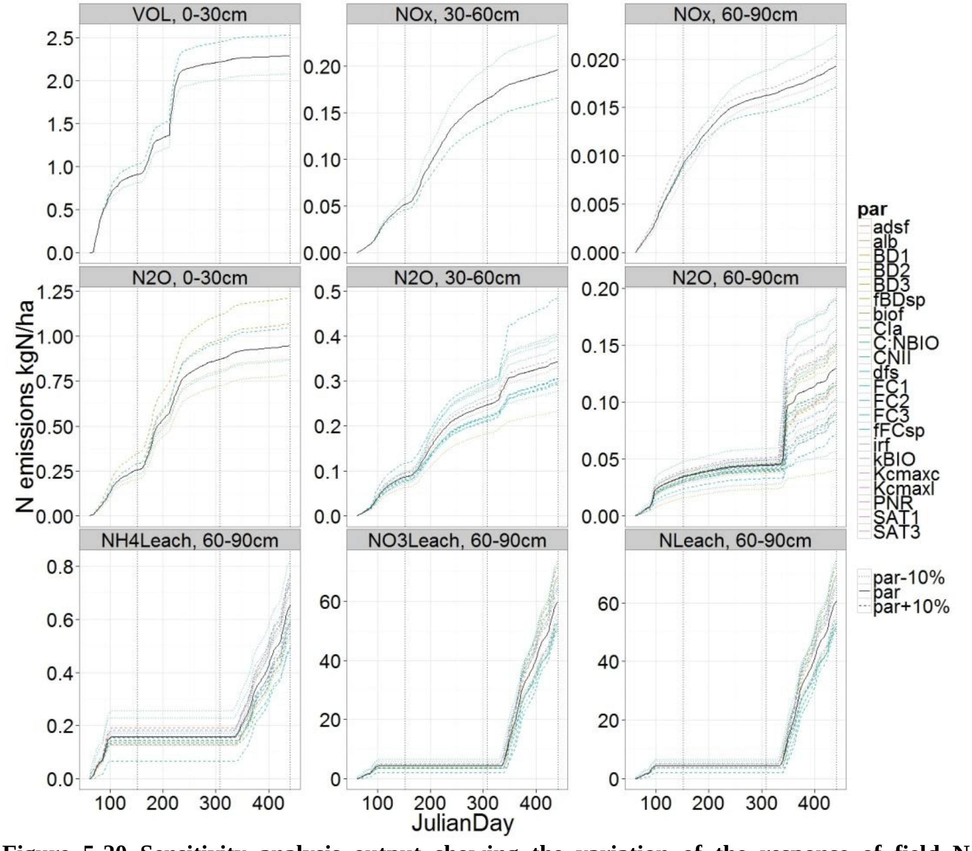

Figure 5-20 Sensitivity analysis output showing the variation of the response of field N emissions (ammonia volatilisation, *VOL*; nitric (*NOx*) and nitrous (*N2O*) oxide emissions and respectively ammonium, nitrate and total nitrogen leaching (*NH4Leach*, *NO3Leach* & *NLeach*) from the different soil layers (top layer 0-30cm, middle layer 30-60cm & lower layer 60-90cm) to a 10% variation on the following parameters: bulk density of all three layers (*BD1, BD2, BD3*), field capacity in all three layers (*FC1, FC2, FC3*), saturation limit of top and bottom layer (*SAT1,SAT3*), adsorption factor (*adfs*), BIO pool fraction of SOM (*biof*), C-N ratio of BIO pool ($C:N_{BIO}$), decay rate of BIO pool (k_{BIO}), depth factor for decomposition (*dfs*), potential nitrification rate (*PNR*), initial abstraction coefficient for runoff (C_{Ia}), curve number for average moisture content (CN_{II}), albedo (*alb*) and maximum crop Kc factor for wet soils during cauliflower and leek cultivation regarding evapotranspiration (K_{Cmaxc} & K_{Cmaxl}).

Table 5-12: Sensitivity analysis output presenting the CV ratios (S_t) regarding the response of field emissions (ammonia volatilisation (NH_3), nitric (NO_x) and nitrous (N_2O) oxide emissions, soil water percolation and nitrogen leaching (Perc, Nleach) from the different soil layers (top layer 0-30cm (=1), middle layer 30-60cm (=2) & lower layer 60-90cm (=3)) to a 10% variation on the following parameters: bulk density of all three layers (BD1, BD2, BD3), field capacity in all three layers (FC1, FC2, FC3), saturation limit of top and bottom layer (SAT1,SAT3), adsorption factor (adfs), BIO pool fraction of SOM (biof), C-N ratio of BIO pool ($C:N_{BIO}$) and the decay rate of BIO pool (k_{BIO}). Each combination of response variable with parameter was evaluated for the three consecutive years 2009-2011 (listed beneath each other), yet only values are listed if the response was sensitive to the respective parameter in the year of evaluation.

	RO	Perc	N leach	NH_3 1	NO_x 2	NO_x 3	N_2O 1	N_2O 2	N_2O 3
BD_1	1.5	1.4	1.5						
	1.2	1.4	1.5						
	1.2	-	1.4						
BD_2								2.3	
								2.1	
								2.7	
BD_3									**5.4**
									4.4
									7.5
FC_1	2.2	**5.3**	**5.3**	1.2			1.1	1.1	**3.4**
	1.6	**5.3**	**5.3**	-			-	1.3	**2.9**
	1.6	1.7	1.2	-			-	1.2	**3.9**
FC_2			1.7					2.5	1.3
			1.7					1.8	1.1
			-					2.9	2.3
FC_3		2.3	2.1						**3.8**
		2.3	2.1						**3.3**
		-	-						**5.6**
SAT_1	1.6	1.6	1.8						1.7
	1.2	1.6	1.8						1.6
	1.2	-	-						2.6
SAT_3									-
									-
									1.4
alb									-
									-
									1.4
biof			-						
			-						
			1.7						
$C:N_{BIO}$			-						-
			-						-
			1.8						1.1
k_{BIO}			-						
			-						
			1.3						

Table 5-12 (Continued) Sensitivity analysis output presenting the CV ratios (S_t) regarding the response of field emissions (ammonia volatilisation (NH_3), nitric (NO_x) and nitrous (N_2O) oxide emissions, soil water percolation and nitrogen leaching (Perc, Nleach) from the different soil layers (top layer 0-30cm (=1), middle layer 30-60cm (=2) & lower layer 60-90cm (=3)) to a 10% variation on the following parameters: depth factor for decomposition (dfs), potential nitrification rate (PNR), initial abstraction coefficient for runoff (C_{Ia}), curve number for average moisture content (CN_{II}), albedo (alb) and maximum crop Kc factor for wet soils during cauliflower and leek cultivation regarding evapotranspiration (K_{Cmaxc} & K_{Cmaxl}). Each combination of response variable with parameter was evaluated for the three consecutive years 2009-2011 (listed beneath each other), yet only values are listed if the response was sensitive to the respective parameter in the year of evaluation.

	RO	Perc	N leach	NH_3 1	NO_x 2	NO_x 3	N_2O 1	N_2O 2	N_2O 3
			-		1.3	-		1.1	-
dfs			-		1.8	1.3		1.7	-
			1.8		1.	1.4		1.6	1.4
			2.0						
adsf			2.0						
			1.7						
			-						
PNR			-						
			1.1						
	2.6	1.0	1.2					-	1.2
CN_{II}	**3.5**	1.0	1.2					-	1.1
	4.0	1.8	1.2					1.1	**4.1**
	1.2		-						-
C_{Ia}	1.5		-						-
	1.7		1.1						2.4
									-
Kc_{mc}									-
									1.3
		-							-
Kc_{ml}		-							-
		1.1							**3.8**

Chapter 6. Model validation

The ultimate model performance was evaluated under different conditions outside the calibration environment. The accuracy of the model was validated in twofold. Two consecutive years of a cauliflower-leek rotation under the N dose 3 rate were simulated with the model and compared with the respective observations. The same objective was set regarding four different N dose rates for the rotation cycle in 2009.

6.1 Validation for two consecutive years

6.1.1 Model input

A few different settings were applied compared to the calibration setup (see section 5.1) and addressed in the following sections as well as an overview of the input and output for the validation years 2010-2011.

6.1.1.1 Simulation control settings

The reference date for the simulation was set at the 1st of January 2010. The simulation started at the 17th of March 2010, the planting date of the cauliflower and ended at the 2nd of March 2012, 716 days later when the next rotation cycle started.

6.1.1.2 Weather

Recordings of the weather during the validation years are presented in Figure 6-1. Daily solar radiation varied from 0.4 to 29.6 MJ m^{-2} day^{-1}, with an average of 10.3 MJ m^{-2} day^{-1} in 2010 and 10.4 MJ m^{-2} day^{-1} in 2011, which was very similar to the 2009 data. The total rainfall amounted up to 871 mm in 2010 and 749 mm in 2011, with a wet autumn in 2010 with 50.8% of the annual rainfall and a wet summer in 2011 with 42.8% of the annual rainfall. The average daily air temperature varied between -6.3 and 27.5°C with maxima in July and August, while December and February were the coldest months in 2010 and 2011 respectively. The average relative humidity ranged from 46.3% during summer till 96.2% during winter. Average wind speed at 2m height maintained 1.6 m s^{-1} over the full cycles.

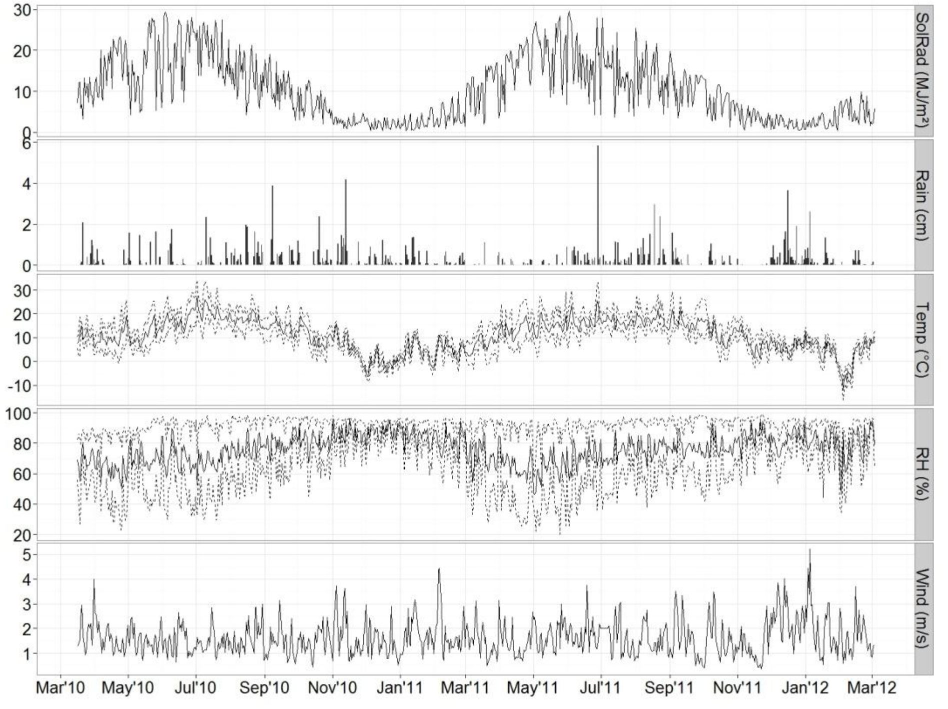

Figure 6-1 Daily weather input data for the validation years 2010-2011 including relative humidity (RH, %), precipitation or rain (cm day^{-1}), solar radiation (SolRad, MJ m^{-2} day^{-1}), air temperature (Temp, °C) and wind speed at 2m height (Wind, m s^{-1}). Dashed lines represent daily minimum and maximum values regarding humidity and temperature.

6.1.1.3 Soil profile properties

Most soil characteristics like texture, pH, organic carbon content (*OC*) and cation exchange capacity (*CEC*) were taken from the measurements at the start of 2009. Of the water content characteristics, only the field capacity (*FC*) was slightly adjusted in accordance with the soil state at the end of the calibrated cycle as the soil undergoes small changes over the year due to soil preparation and irrigation. Initial contents of water (*SWC*) and nitrogen (*N*) were measured as described in the experimental setup (see Chapter 2). These properties different from calibration, are summarized in Table 6-1.

Table 6-1 Soil physical and chemical data for the profile at the start of validation years 2010-2011 (Layer thickness (LT), soil water content at field capacity (FC) and initial level (SWC), soil mineral nitrogen content (N_{min})).

Layer	LT [cm]	FC [cm³/cm³]	SWC [cm³/cm³]	N_{min} [kg/ha]
1	10	0.28	0.35	18.5
2	20	0.28	0.35	37
3	30	0.33	0.34	36
4	30	0.33	0.33	36

6.1.1.4 Crop management

Again the crop growth started after transplanting the cauliflower seedlings in 2010, followed by similar fertilizer application schemes in both rotation cycles according to the N dose 3 rate. The characteristics of the seedlings were similar to the ones from the calibration period (see Table 5-2) as were the planting densities of 4 and 18.18 plants m² for respectively cauliflower and leek.

Crop characteristics

The planting dates of cauliflower and leek were the 17th and 10th of March for cauliflower and the 24th and 17th of June for leek in respectively 2010 and 2011. While planting dates were set as in the experiment, their respective harvesting date was simulated in relation to the accumulated thermal time (ATT) from the calibration year. This resulted in a predicted developmental stage (DVS) that was compared with the estimated DVS based on observed ATT and cultivation length as shown in Figure 6-2and presented in Table 6-2. Compared to 2009, the growth cycle of cauliflower was 4 days shorter in 2010 and even 15 days in 2011. The prediction approached the observed growth cycle by 1 and 2 days for the respective validation years, which is very close considering that the harvest during the experiment took several days around the defined dates. In 2010 and 2011 cauliflower reached maturity respectively 10.9 and 20.2 degree days earlier or 1.6 and 3% less compared to 2009. Yet, curd initiation had an opposite offset of +18.4 and -83.1 degree days which resulted in predictions of curd initiation 5 days later and 9 days earlier than observed in 2010 and 2011 respectively. The latter does show some uncertainty as it was hard to determine without too much crop destruction if 50% of the plants started with curd growth. The observed leek cultivation in the validation years were respectively 15 and 5 days longer, reaching mature shafts after 1934 and 1884 degree days or 2.8 and 0.1% more than calibrated. The model predicted an earlier harvest by 9 days in 2010 while in 2011 harvest would have been 5 days later.

Table 6-2 Overview crop related management characteristics as observed in the respective years and predicted based on the calibrated year.

	2010		2011	
	Cauliflower	**Leek**	**Cauliflower**	**Leek**
Planting	17/03/2010	24/6/2010	10/03/2011	17/6/2011
Curd initiation	7/05/2010	-	4/05/2011	-
(predicted)	(+5 days)		(-9 days)	
Harvesting	11/06/2010	18/11/2010	24/05/2011	27/10/2011
(predicted)	(+1 day)	(-9 days)	(+2 days)	(+5 days)
ATT mature	660.1	1934.2	650.8	1826.1
(predicted)	(671)	(1881.9)	(671)	(1883.6)
ATT curd	322.9	-	424.4	-
(predicted)	(341.3)		(341.3)	
Growth length	86 (51+35)	147	75 (55+20)	133
(predicted)	87 (57+30)	138	77	138

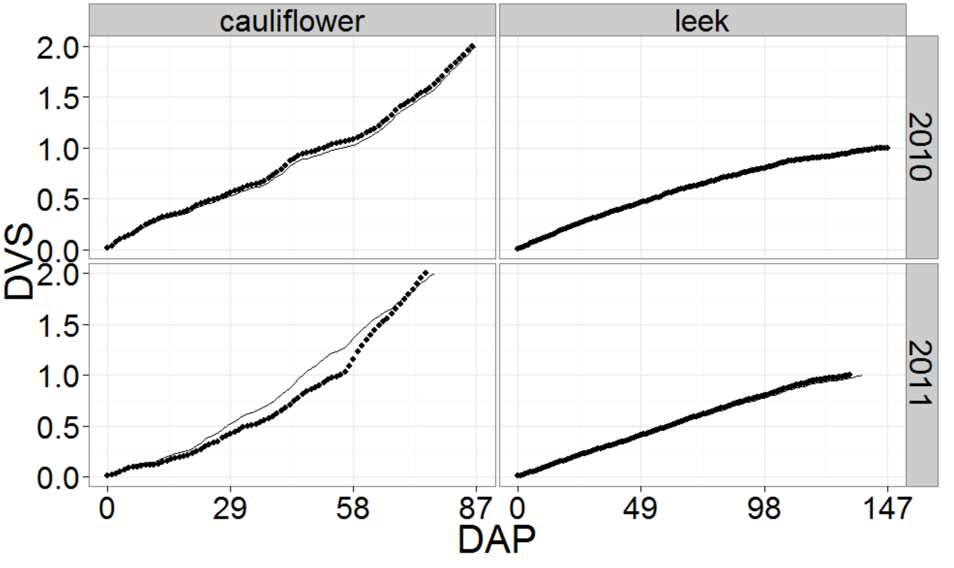

Figure 6-2 Developmental stage (DVS) of both crops as a function of days after planting (DAP) as calculated daily based on the observations in the validation years 2010-2011 (dotted lines) and on the calibrated data from 2009 (solid lines).

Irrigation and fertilizer application

In 2010 no additional water was applied, while the year after 78.2 mm was irrigated along the second half of cauliflower cultivation. The irrigation scheme as well as the fertilizer application is presented in Figure 6-3.

Like in the calibrated cycle three applications of inorganic fertilizer were applied on the soil surface each year: 124, 108 and 106 kg N ha^{-1} in 2010 and 105, 75 and 96 kg N ha^{-1} in 2011, respectively at cauliflower planting, 7 weeks later and 5 weeks after the leek planting date. Compared to 2009, 50 and 16% more N fertilizer was applied in the consecutive years for cauliflower while amounts were similar for leek. Also, one week after cauliflower harvest, incorporation of its crop residue added 1166 kg C ha^{-1} and 103.6 kg N ha^{-1} in 2010 and 890.8 kg C ha^{-1} and 61.4 kg N ha^{-1} in 2011 to the top 20cm soil. Furthermore, at the harvest of cauliflower and leek roots from the respective crops remained in the soil distributed over the soil root depth set to decompose. Amounts were assumed similar to 2009 due to lack of measurements.

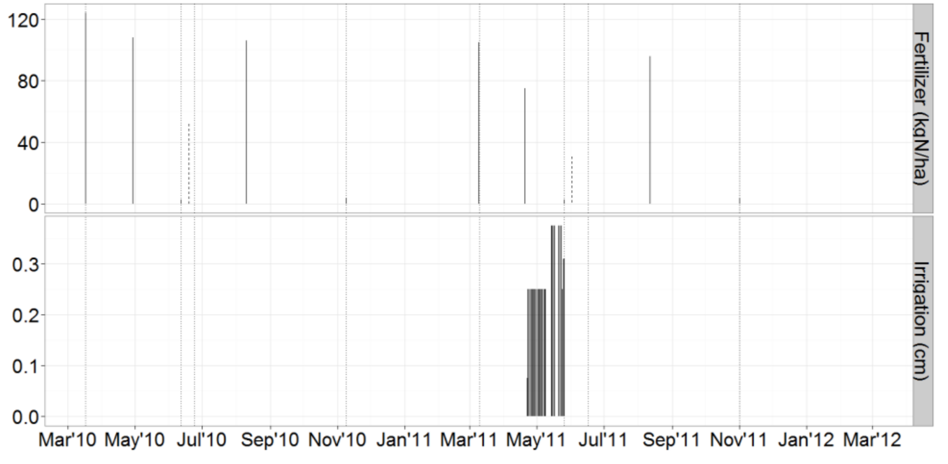

Figure 6-3 Overview of the fertilizer application and irrigation management during the crop rotation of cauliflower and leek in the years 2010-2011 (dotted lines represent the start-end dates of the respective crops; in the upper graph the solid bars represent synthetic or inorganic fertilizer application and the dashed bars represent the organic fertilizer through root and crop residue incorporation at harvest and one week later respectively).

6.1.2 Model performance statistics

Similar to the calibration (see section 5.2) , the model performance was evaluated through both graphical techniques and quantitative statistics, including the time series plot of the constituent of interest, the plots of observed versus simulated output complemented by the set of statistical indicators, i.e. Nash-Sutcliffe efficiency (NSE), RMSE- observations standard deviation ratio (RSR) and percent bias (Pbias). The reliability of the model is thus tested for conditions outside the calibration environment as weather, cultivation dates and fertilizer rates differ.

Ultimate performance rating was achieved according to the same thresholds for calibration. Due to the different conditions as mentioned above, satisfying statistics (NSE > 0.5, RSR < 0.7 and Pbias<25%) would signify a good validation.

For the validation results an overview of all output is given in Table 6-3.

6.1.3 Validation output

The model output is in accordance with the calibration results and relates to the four main state variables concerning (1) the crop biomass including its nitrogen content, (2) the soil water content, (3) the soil temperature and (4) the soil nitrogen content. Their simulation was evaluated in accordance with the observations, followed by an overview of the unobserved processes which interacted with them.

6.1.3.1 Crop biomass and nitrogen uptake

Figure 6-4 shows the two consecutive growth rotation cycles of cauliflower and leek in 2010-2011. The boxplots again represent the observed biomass production at each of the destructive sampling days. The results along with the performance statistics are presented in Table 6-3. Observations in 2010 and 2011 showed shorter cultivation lengths for cauliflower, by 4 and even 15 days, which was also predicted by the model in accordance with the ATT. Yet, the cauliflower growth behaved differently according to the measurements and the corresponding simulations. While the observed shoot yield changed by -5% in 2010 and +7% in 2011 compared to the observations in 2009, the model predicted opposite results, although still within the range of observed yields. The observed difference between the years was even higher on the cauliflower curd with -32% and +25% respectively, while the amount of leaves and stems remained rather equal. The proportional share of dry matter for each plant organ corresponded however better between the observations and the model predictions.

Leek growth was also variable in the consecutive years. Compared to 2009, a longer cultivation length in 2010 and similar in 2011 yielded lower amounts, with an extreme decrease of 40% in 2011. Where the model predicted a lower yield in 2010, although slightly higher as observed despite less growing degree days, predicted yield in 2011 was similar as in 2009 and did not expect the observed production decrease. Regarding plant organs, a slight overestimation of the shaft in 2010 caused the difference in observed and predicted yield, while both shaft and leaves of the leek observed in 2011 were far below the simulated values.

Next, the simulated nitrogen uptake was close to the observations as shown in Figure 6-5 and Table 6-3. At the sampling moment in 2011 before leek harvest however, the offset might suggest an error occurred during the nitrogen analysis as amounts were lower than the previous sampling measurements and do not correspond with the trend observed in 2010.

For the leek crop, also the shaft diameter and length was validated in 2010-2011. As there simulations are solely dependent on ATT, predictions follow the calibrated results. This resulted in fairly good estimations with exception of an overestimation regarding the average diameter of the leek in 2011.

As with calibration, the approximation of the model predictions with the observations was quantified by the performance statistics as shown in Table 5-6. Overall fair to even very good ratings for NSE, RSR and Pbias were achieved for both the crop growth in the consecutive years. Poor results were obtained for the 'Fruit' dry matter, although close to the thresholds, and the shaft's diameter of leek in 2011.

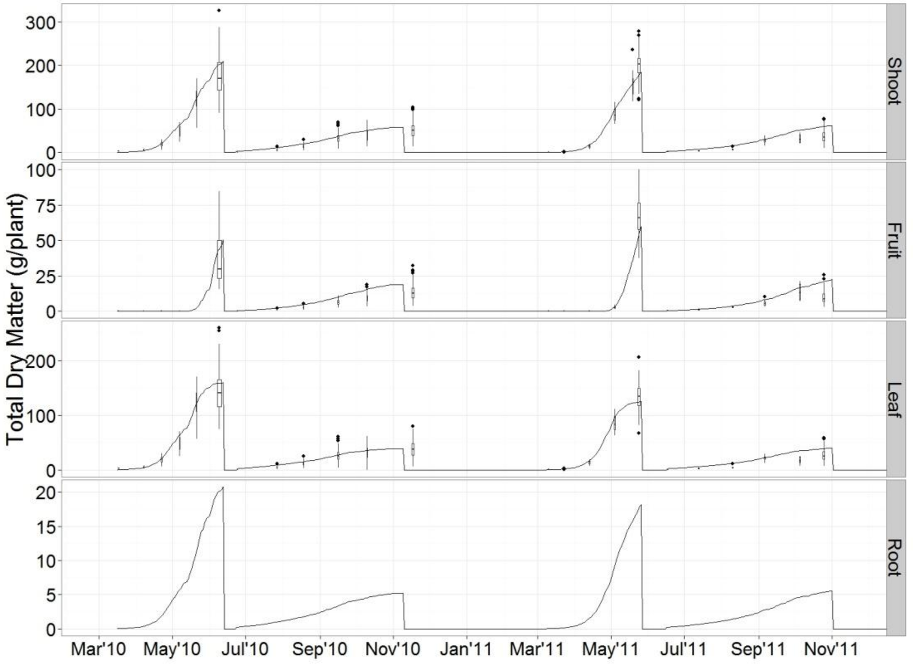

Figure 6-4 Validation output of the biomass or dry matter for 2 rotations of cauliflower and leek in 2010-2011, i.e. for the shoot, the fruit, the leaves (including the stem for cauliflower) and the roots. Boxplots denote the measurements (the box shows the 1st and 3rd quartile around the median, whiskers are extended to values within the 1.5*box length or 1.5*interquartile range; outliers are shown by black dots) and simulated growth is presented by the solid line.

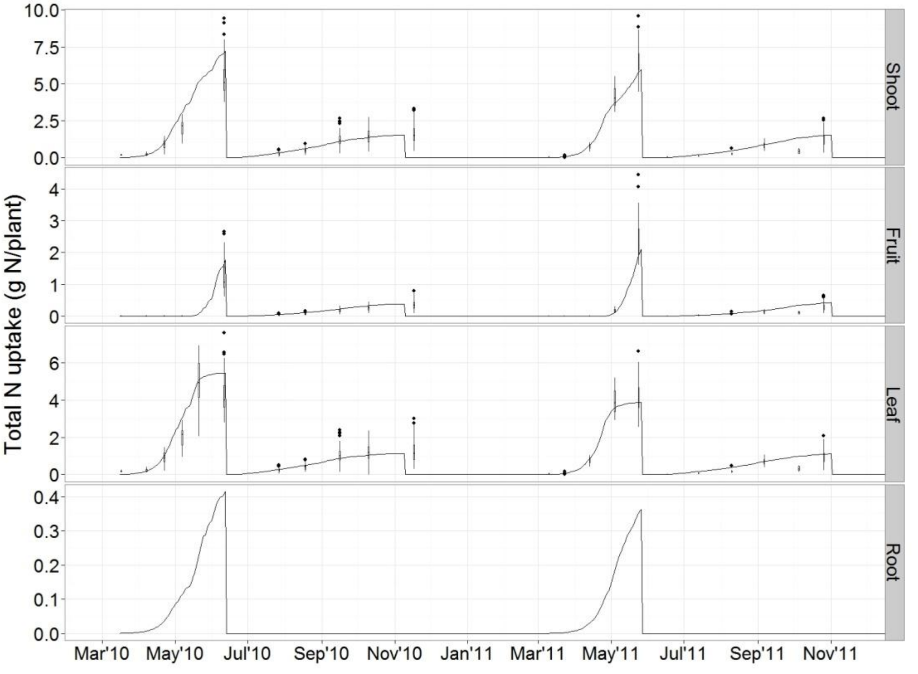

Figure 6-5 Validation output of the N uptake for cauliflower and leek in 2010-2011, i.e. for the shoot, the fruit, the leaves (including the stem for cauliflower) and the roots. Boxplots denote the measurements (the box shows the 1st and 3rd quartile around the median, whiskers are extended to values within the 1.5*box length or 1.5*interquartile range; outliers are shown by black dots) and simulated N uptake is presented by the solid line.

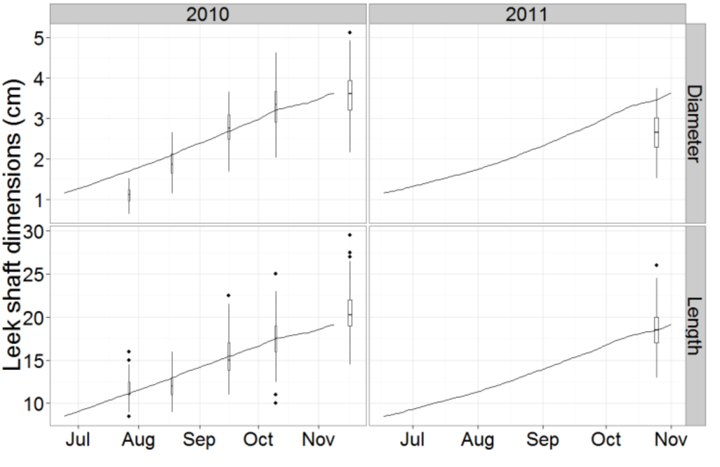

Figure 6-6 Validation of the leeks shaft properties, i.e. the diameter and length in 2010-2011. Boxplots denote the measurements (the box shows the 1st and 3rd quartile around the median, whiskers are extended to values within the 1.5*box length or 1.5*interquartile range; outliers are shown by black dots) and simulation is presented by the solid line.

Table 6-3 Overview of the validation output in 2010-2011 and model performance statistics (bold, regular and *(*) values indicate respectively a poor, satisfactory and (very) good rating).

		$\overline{O_i}$	sd_{O_i}	S_h	NSE	RSR	Pbias
	Year	**Cauliflower Leek**		**at harvest**		**whole rotation cycle**	
Dry matter (g DM plant^{-1})							
Shoot	2010	179.0 51.5	43.6 18.0	209.9 57.5	0.85**	0.39**	14.29*
	2011	201.3 36.7	28.4 14.2	184.5 61.8	0.87**	0.37**	14.27*
Fruit	2010	36.2 13.3	15.9 5.1	50.6 18.9	**0.47**	**0.73**	**43.85**
	2011	67.7 9.6	12.9 4.0	59.9 22.2	0.78**	0.47**	22.82
Leaf	2010	144.6 38.2	34.5 14.6	159.2 38.5	0.87**	0.36**	6.95**
	2011	133.6 27.1	23.0 10.5	124.7 39.6	0.87**	0.36**	11.14*
Root	2010	- -	- -	20.8 5.2	-	-	-
	2011	- -	- -	18.2 5.6	-	-	-
Nitrogen content (g N plant^{-1})							
Shoot	2010	5.6 1.6	1.4 0.6	7.2 1.5	0.71*	0.54*	10.20*
	2011	6.5 1.2	1.0 0.5	6.0 1.5	0.91**	0.29**	1.36**
Fruit	2010	1.3 0.4	0.5 0.1	1.8 0.4	0.59	0.64	**26.6**
	2011	2.4 0.3	0.6 0.1	2.1 0.4	0.88**	0.35**	-0.19**
Leaf	2010	4.4 1.2	1.1 0.5	5.4 1.1	0.79**	0.46**	6.17**
	2011	4.1 1.0	0.8 0.4	3.9 1.1	0.88**	0.34**	1.95**
Root	2010	- -	- -	0.4 -	-	-	-
	2011	- -	- -	0.4 -	-	-	-
Leek shaft (cm)							
Diameter	2010	3.6	0.6	3.6	0.73*	0.52*	4.57**
	2011	2.7	0.5	3.6	**-3.52**	**2.13**	**35.45**
Length	2010	20.5	2.5	19.1	**0.49**	**0.72**	-5.13**
	2011	18.5	2.0	19.1	0.52	0.69	0.27**

Additionally to the model performance statistics, the graphic representation in Figure 6-7 shows how well the data of observations versus simulations fit the 1:1 line.

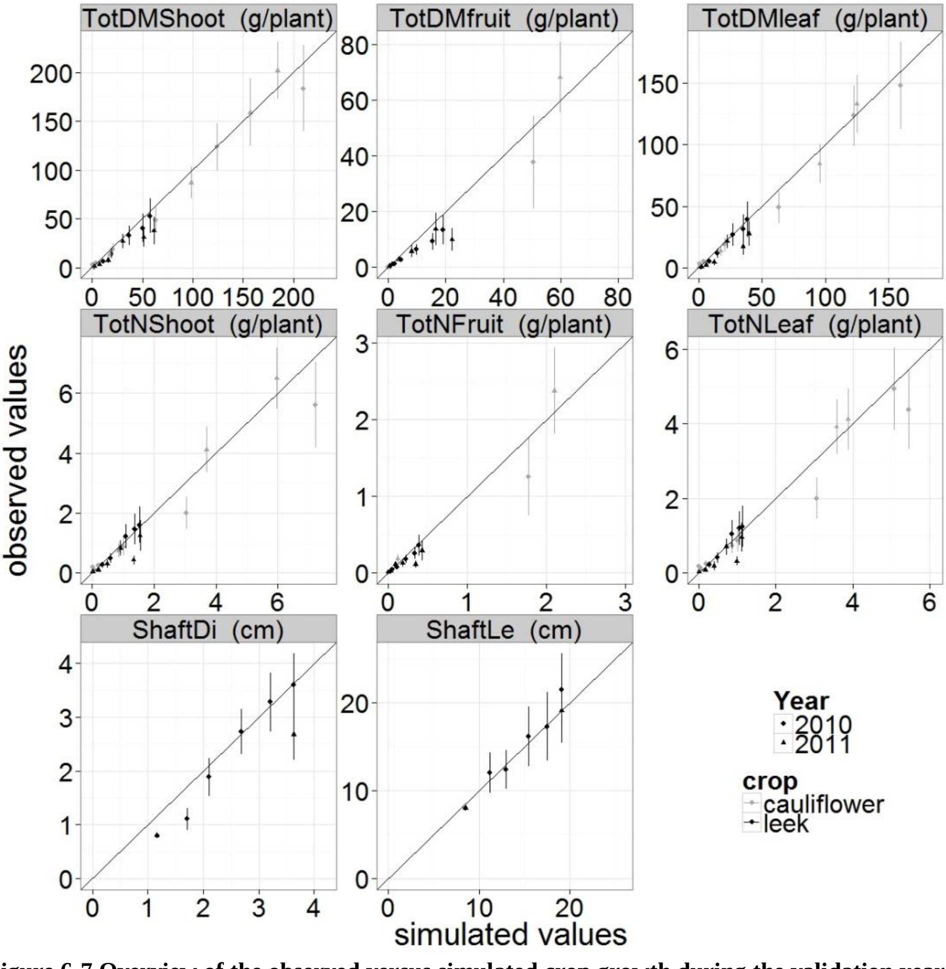

Figure 6-7 Overview of the observed versus simulated crop growth during the validation years 2010 (♦) and 2011 (▲) regarding crop dry matter (*TotDM*) and nitrogen content (*TotN***) for *shoot*, *fruit* and *leaf* for both cauliflower (black) and leek (grey); as well as stem or shaft properties, i.e. the diameter (*ShaftDi*) and length (*ShaftLe*) of the leek crop. Error bars denote the range of observed values around the average.**

6.1.3.2 Soil water content

The soil water content was simulated and compared with the observations from the TDR sensors in two consecutive soil layers of 30 cm thickness. As shown in Figure 6-8 the soil water content decreases in both soil layers during the cauliflower growing periods while for leek this differs each year. As the crop matures, water is taken up to meet the transpiration demands, but might be (partly) compensated by increased precipitation as occurred during leek growth in the summers/autumns of 2010-2011. The decreases in the lower soil layer were more pronounced during cauliflower cultivation compared to 2009 despite lower root density. In 2011 at the end of cauliflower cultivation irrigation (bars) was applied. One peculiarity occurred during the fallow period between the two cycles were a peak in soil water content was measured but was not predicted by the model. As no extreme precipitation was observed, a malfunction of TDR equipment might have been the cause.

Ultimately, this resulted in fair to very good performance ratings regarding NSE, RSR and Pbias values for the whole simulation (see Table 6-4).

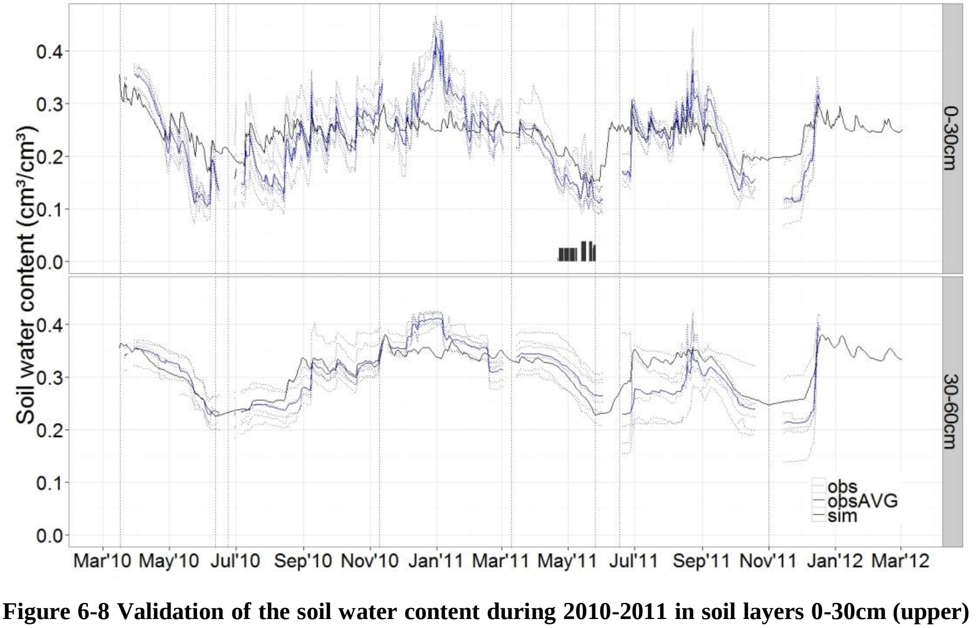

Figure 6-8 Validation of the soil water content during 2010-2011 in soil layers 0-30cm (upper) and 30-60cm (lower) with observations (*obs, blue dotted lines)*, their average value (*obsAVG, blue solid line*) and the simulated values (*sim, black solid line*). Vertical dashed lines represent the growing periods of cauliflower and leek. Black bars indicate the irrigation scheme

Table 6-4 Validation output of the soil water content in two consecutive soil layers of 30cm in 2010-2011 with respective model performance statistics (bold, regular and $*^{(*)}$ values indicate respectively a rating of poorly, satisfactory and (very) good).

	$\overline{O_i}$	sd_{O_i}	$\overline{S_i}$	NSE	RSR	Pbias
0-30cm	0.23	0.07	0.24	0.60	0.63	3.58**
30-60cm	0.30	0.05	0.31	0.69*	0.55*	1.84**

The graphical representation of the model performance regarding soil water content (SWC) is shown in Figure 6-9 where observed data was plotted against the simulated data to visualize how well these data would fit the 1:1 line.

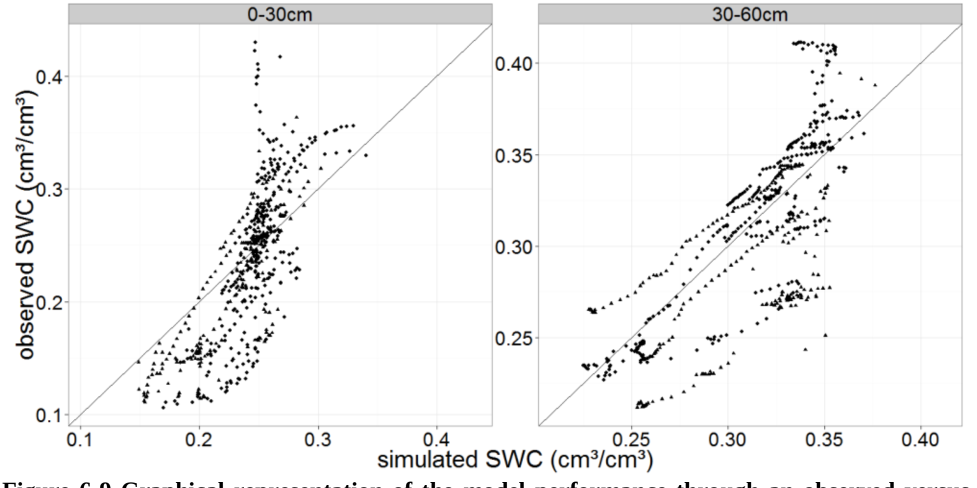

Figure 6-9 Graphical representation of the model performance through an observed versus simulated soil water content plot in two consecutive 30cm soil layers during the validation years 2010 -2011.

6.1.3.3 Soil temperature

Also for the years 2010-2011 simulations and observations of the soil temperature at 15 and 45cm from the surface were compared. The model successfully simulated the overall temporal pattern for soil temperatures at both depths, as shown in Figure 6-10and confirmed by the performance statistics presented in Table 6-5 and visualized in Figure 6-11. A very small overestimation of soil temperature, especially when crops are mature, was confirmed during the validation years. As mentioned before, discussing the calibration, this overestimation could possibly be avoided by introducing a plant shading factor in the future.

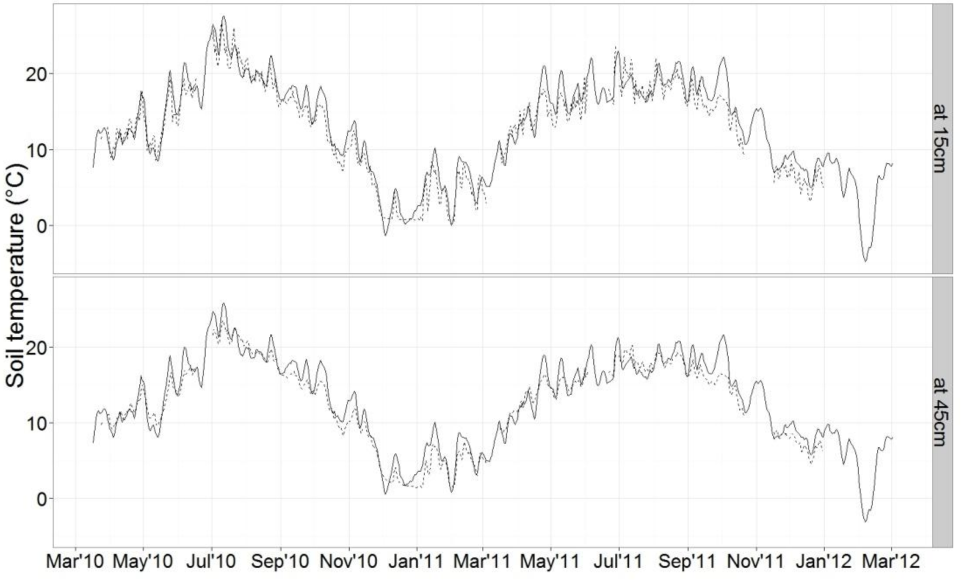

Figure 6-10 Validation of the soil temperature at 15 (upper) and 45cm depth (lower) with observations (dashed lines) and simulated values (solid lines) during 2010-2011.

Table 6-5 Validation output of the soil temperature at two soil depths in 20010-2011 with respective model performance statistics (bold, regular and *(*) values indicate respectively a rating of poorly, satisfactory and (very) good)).

	$\overline{O_i}$	sd_{O_i}	$\overline{S_i}$	NSE	RSR	Pbias
Soil temperature (°C)						
At 15cm	12.7	6.2	12.9	0.94**	0.25**	7.23**
At 45cm	12.5	5.5	12.6	0.94**	0.24**	5.78**

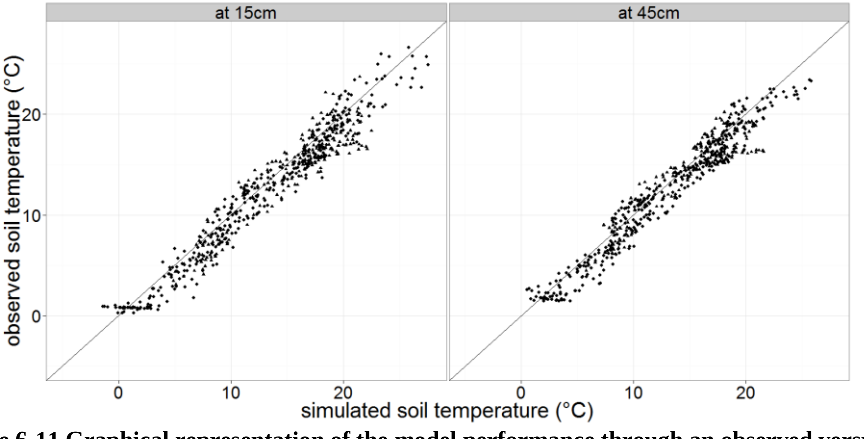

Figure 6-11 Graphical representation of the model performance through an observed versus simulated soil temperature plot at two soil depths during the validation years 2010-2011.

6.1.3.4 Soil mineral nitrogen content

Simulation of the soil mineral nitrogen content in two consecutive soil layers of 30 cm, similar to the soil water content, was validated with the observations during the years 2010-2011.

The model did a fair prediction as shown in Figure 6-12, but also revealed some irregularities. As the ammonium content in 2009 was underestimated, the opposite occurred in 2010, while similar propagation was predicted in 2011 for both soil layers. Besides more fertilizer that was applied in 2010, more research is required regarding ammonium adsorption, as mineralisation was similar (see further), and nitrate content was predicted quite well. Only, during leek cultivation the model showed larger nitrogen amounts in the deeper layer than in the upper 30cm while measurements suggest otherwise, especially after the fertilizer application in 2010 and before in 2011. As no exceptional percolation occurred and adjustment of the simulated drain process did not improve the results, this might suggest an adaptation of the leek root distribution. But then again this would change the soil water content which was simulated well and would require changes in all soil water related processes. Simulated uptake of nitrogen by the crop was furthermore higher than observed which does not explain the overestimation of soil nitrate during leek cultivation. A potential increase in denitrification would not transform nitrate in such amounts that the simulation would fall more closely to the observations. The large amount of N observed in the upper layer in 2011 before even fertilizer is applied, suggest doubtful measurements and/or a much higher effect of crop residue incorporation has to be accounted for.
Again the difficult task of model calibration and validation is confirmed due to the complex interactions of multiple processes to which the different state variables respond, especially if observed data is highly variable and limited.
Subsequently this resulted in poor performance ratings as presented in Table 6-6 in accordance with the defined thresholds for the NSE, RSR and Pbias statistics.

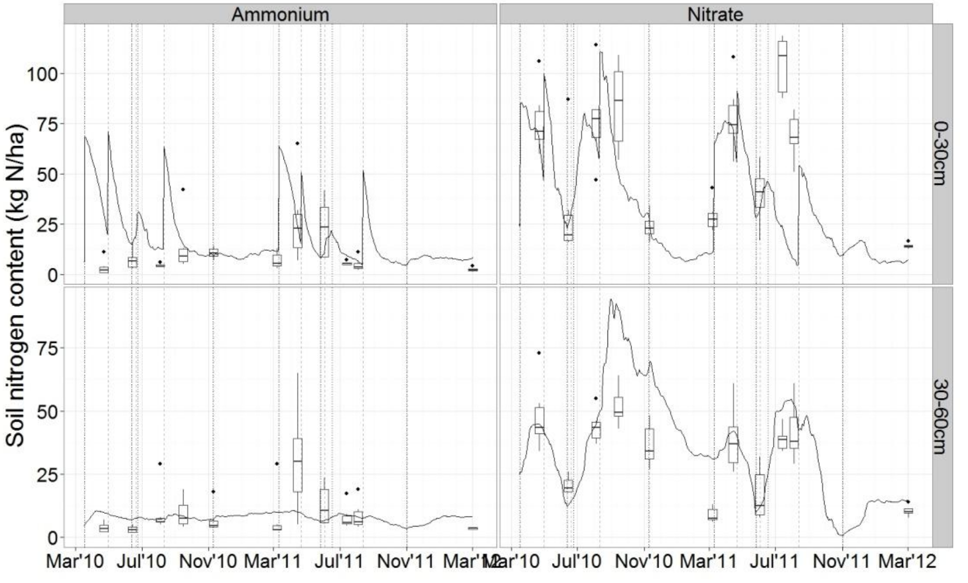

Figure 6-12 Validation of the soil mineral nitrogen content as nitrate and ammonium (in kgN ha^{-1}) in soil layers 0-30cm (upper) and 30-60cm (lower) during the years 2010-2011 with observed values represented by boxplots (the box shows the 1st and 3rd quartile around the median, whiskers are extended to values within the 1.5*box length or 1.5*interquartile range; outliers are shown by black dots) and simulated growth presented by the solid line. Vertical dashed lines represent the growing periods of cauliflower and leek.

Table 6-6 Validation output of the soil mineral nitrogen content (for ammonium and nitrate separately) in two consecutive soil layers of 30cm in the years 20010-2011 with respective model performance statistics (bold, regular and $*^{(*)}$ values indicate respectively a rating of poorly, satisfactory and (very) good)).

	$\overline{O_i}$	sd_{O_i}	$\overline{S_i}$	NSE	RSR	Pbias
Soil ammonium content (kg N ha^{-1})						
0-30cm	11.1	12.0	13.6	**-0.25**	**1.12**	22.91
30-60cm	9.7	10.6	8.1	**0.0034**	**1.00**	-16.48
Soil nitrate content (kg N ha^{-1})						
0-30cm	54.7	31.5	35.1	**-0.11**	**1.05**	**-34.89**
30-60cm	31.1	16.8	39.7	**-0.22**	**1.11**	**27.69**

6.1.3.5 Other soil processes

Model output during the validation period 2010-2011 regarding unobserved processes including the nitrogen emissions are presented in Figure 6-13 to Figure 6-15 similar to the flow output at calibration. An overview of the quantitative soil water and nitrogen flows is listed through the respective balances in Table 6-7 and Table 6-8.

Water flow

During the validation years, rainfall interception amounted up to an average of 9% of the precipitation and additional irrigation. Surface runoff accumulated up to 15% with peaks at heavy rainfall. The total soil water content decreased by 11% after 359 days from the start of cauliflower but remained the same at the end of the 2nd cycle. An average of 453mm evapotranspired of which 64% through the plant and the rest from the soil. Meanwhile, soil water percolated again deeply out of reach for plant uptake at the early stages of cauliflower cultivation, but especially during the fallow period over winter by 78%. In 2011 even during leek cultivation in September water leached out as relative more rain fell on the already wet soil. This water outflow in the groundwater table mounted up to an average of 21% of the water present in the soil with the cumulative addition of rain and irrigation.

Table 6-7 Simulated soil water balance for the validation period.

Water flow (cm)	2010	2011
Rain	+87.09	+74.99
Irrigation	+0	+7.82
Interception	-9.22	-6.40
Runoff	-13.52	-12.65
Net SWC_{tot} change	+3.53	+0.08
Soil evaporation	-15.36	-17.14
Plant transpiration =water uptake	-29.17	-28.91
Deep percolation	-23.34	-17.63
Balance	≈0	≈0

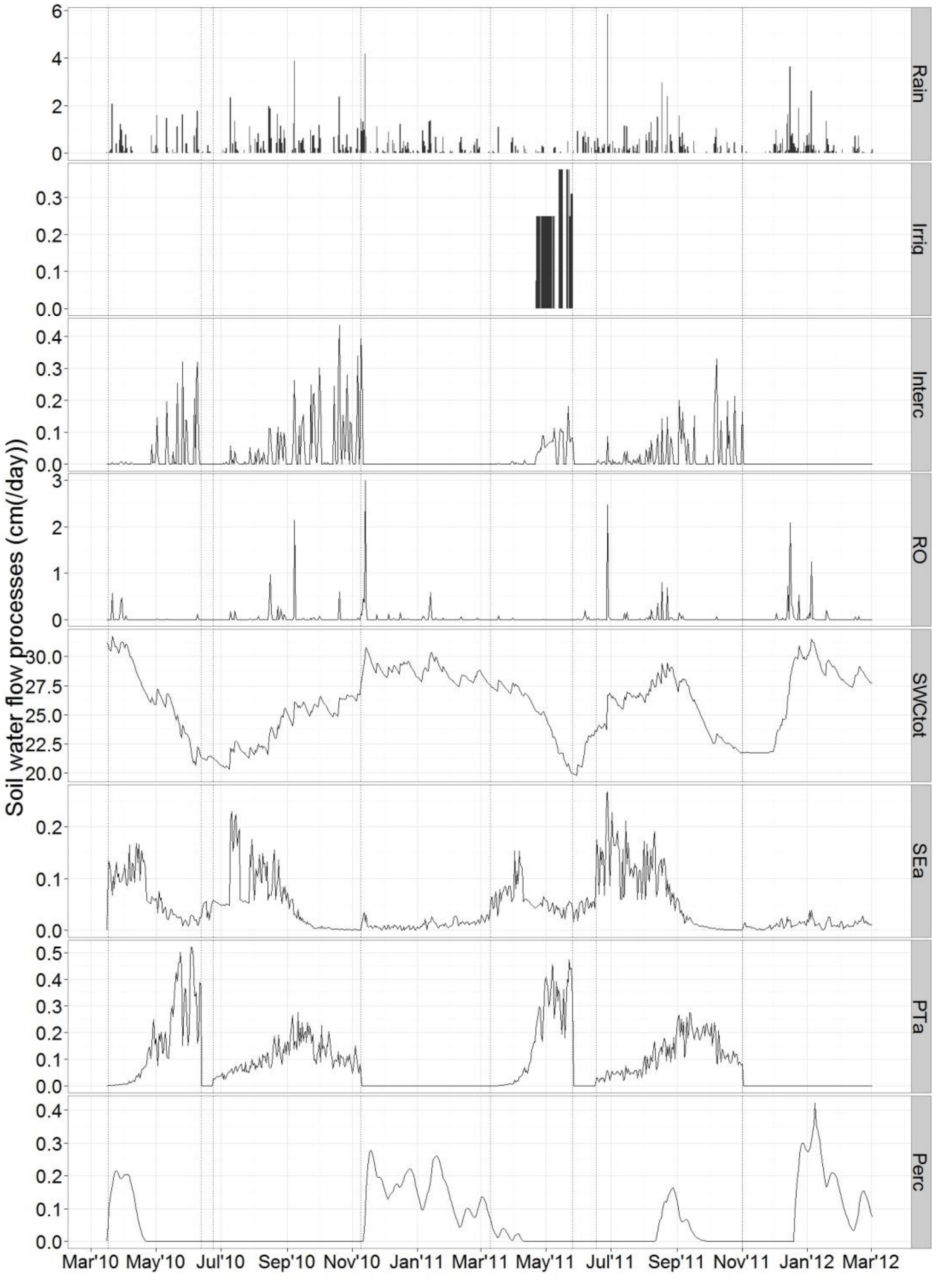

Figure 6-13 Overview of the soil water flow processes affecting the total soil water content (*SWCtot, cm*) during the validation years 2010-2011: rain, irrigation (*Irrig*), interception (*Interc*), runoff (*RO*), actual soil evaporation (*SEa*), actual plant transpiration (*PTa*) and soil water percolation (*Perc*): all in cm day^{-1}.

Nitrogen flow

The soil organic matter (SOM) pools mineralized again with a daily average of 1 kg N ha^{-1} and showed peaks of organic N after crop residue is incorporated in the top 30cm soil. Mineralisation mobilized a minimum of 3.8 kg N ha^{-1} in December 2010 up to a maximum of 85.2 kg N ha^{-1} in August. Overall a yearly average release of 2.5% of organic bounded nitrogen into the free ammonium pool is simulated, without any day of net immobilisation going backwards, similar to the calibration year. Every year inorganic nitrogen fertilizer was added through broadcast application and organic through soil incorporation of crop residue and roots decay after harvest, which let to peaks in the ammonium and nitrate pool and the SOM-N pool respectively. In the two consecutive years, 26% more and 25% less (organic and inorganic) fertilizer was added to the soil compared to 2009, while the model predicted 5% more and 25% less nitrification with the corresponding differences in NO_x and N_2O (68% on average from nitrification) emissions as well. Furthermore, predictions of 1% more ammonia loss in 2010 and 26% less in 2011 showed a countering or supplementing effect of climate and soil conditions to the application of fertilizer. Meanwhile, two to three times more nitrate leaves the soil through denitrification as higher soil water contents over the validation years caused longer anaerobic conditions favouring the release of N_2O (24%) and N_2 (76%). Of the nitrogen uptake by cauliflower and leek respectively 77% and 89% is predicted to be in the form of nitrate. As water percolates deeper into the soil, nitrogen is leached out cumulating up to 77% more in 2010 and equal amounts in 2011 as in the calibrated year of 2009.

Ultimately, with the amount of water leached, concentrations of nitrogen ranged from 16.5 up to 54.1 mg L^{-1} during the early cauliflower cultivation, the fallow periods and even the leek cultivation in 2011.

Table 6-8 Simulated soil nitrogen balance for the validation period.

Nitrogen flow (kgN ha^{-1})	2010	2011
Organic fertilizer	+117.04	+74.83
Mineral fertilizer	+338	+276
Net N_{org} change	+260.1	+200.73
Net N_{min} change	-18.99	+48.21
N uptake	-582.2	-534.02
NH_3 volatilisation	-2.32	-1.7
NO_x (nitrif)	-1.14	-0.82
N_2O ((de)nitrif)	-1.75	-1.43
N_2	-1.52	-1.64
N Leaching	-107.2	-60.17
Balance	≈0	≈0

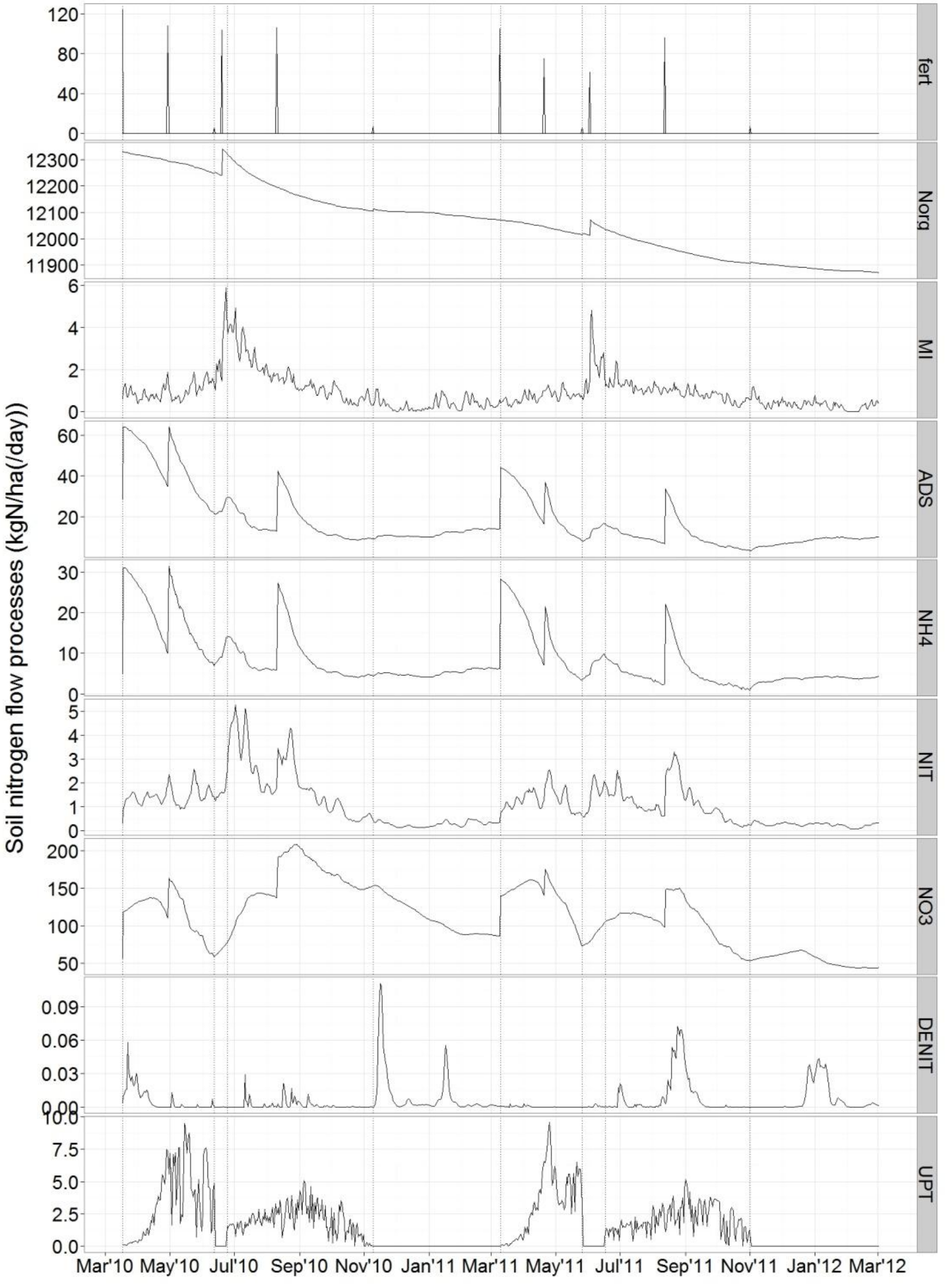

Figure 6-14 Overview of the simulated daily soil nitrogen flow processes (kgN ha^{-1} day^{-1}), i.e. fertilizer application (*fert*), mineralisation (*MI*), nitrification (*NIT*), denitrification (*DENIT*) and soil nitrogen uptake by crops (*UPT*), during the validation period 2010-2011, affecting the total soil nitrogen contents (kgN ha^{-1}) of soil organic nitrogen (N_{org}), free (NH_4) and adsorbed (*ADS*) ammonium and nitrate (NO_3).

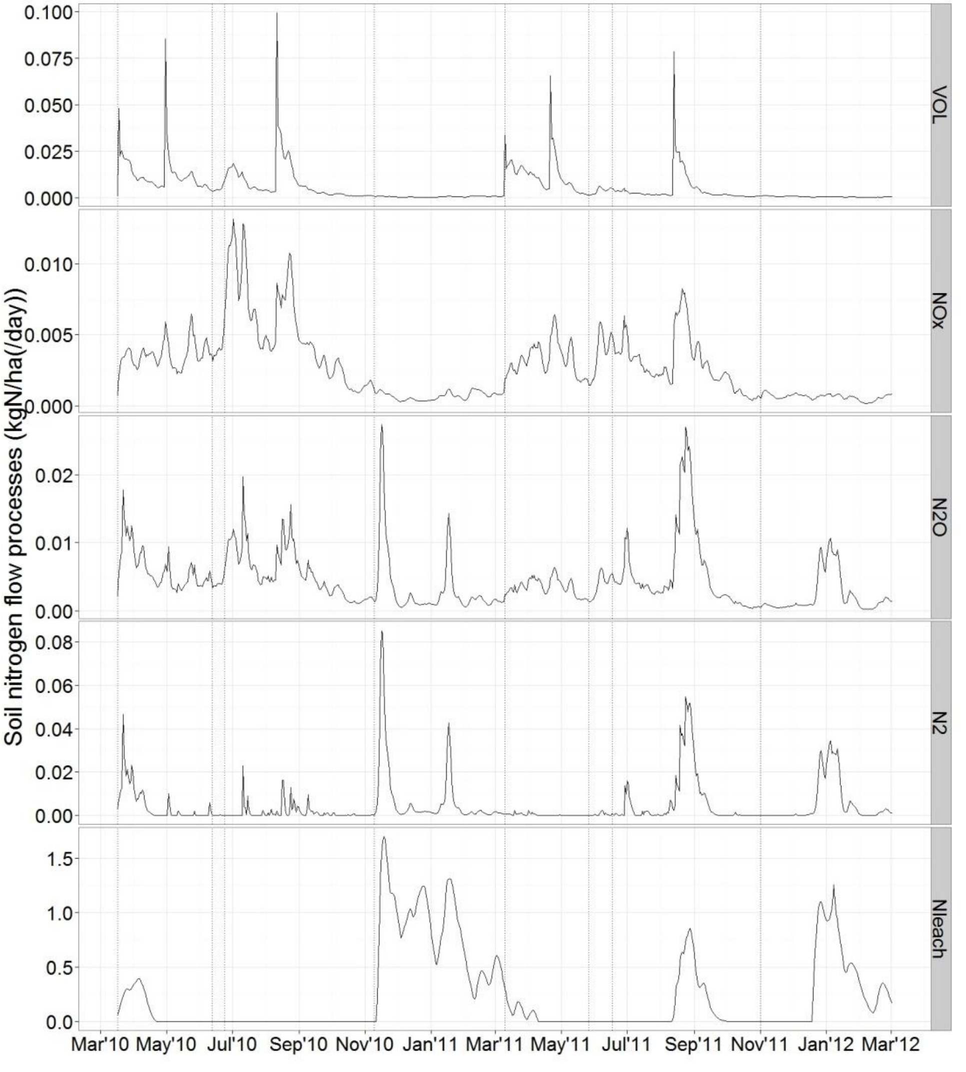

Figure 6-15 Overview of the soil nitrogen emissions (kgN ha^{-1} day^{-1}) affecting the total soil nitrogen content during the validation years 2010-2011: ammonia volatilisation (*VOL*), nitrogen oxide (*NO_x*), dinitrogen oxide (*N_2O*), dinitrogen (*N_2*) and nitrogen leaching (*Nleach*).

6.2 Validation of four N dose rates

As mentioned in Chapter 2, the N dose 3 rate was the recommended rate based on an advisory system assuming optimal photosynthetic capacity. Therefore it was also chosen as rate applied for calibration of the system model assuming no lack of nutrients would occur in order to reach the observed crop yield. As described in Chapter 4, the model integrates a soil deficiency factor representing stress conditions when the supply of water and/or nitrogen does not meet the daily demand of the crop, and subsequently limiting the potential dry matter accumulation. The next validation procedure evaluates if the differences in yield as observed during the experiment under the different N dose rates are correctly predicted by the deficiency factor implementation in the model.

For N doses 1 and 2, the N supply is considered insufficient causing N-stress. This has a detrimental effect on photosynthetic capacity. With N dose 4, the luxury excess of N also is expected to have a, although very small, negative effect due to a combination of higher dark respiration in leaves with higher N content (DeJong, 1982; Hirose et al., 1989) and the small effect of increasing chlorophyll on energy capture near saturation (Björkman, 1981), resulting in a net offset against increased photosynthetic rates (Mooney and Gulmon, 1979). Nevertheless, this negative surplus effect was not implemented in the model. Similar simulations for N dose 3 & 4 were expected (regarding crop yield) and compared with their respective observations to assess to which extent differences would appear.

6.2.1 Crop management

All conditions were taken from the calibration, besides the fertilizer management regarding the applied N dose rate.

Irrigation and fertilizer application

All N dose treatments received equal daily irrigation amounts. To recapitulate (see Table 6-9 and Figure 6-16), two fertilizer amounts were applied during cauliflower cultivation, at the start and 7 weeks later. For leek only one application was given 5 weeks after transplanting. The lowest N dose rates comprised cumulatively 47% and 40% of the reference dose for cauliflower and leek application respectively. This increased up to 74% and 80% for both crops regarding N dose 2. The highest rate applied 28% and 40% more nitrogen for the respective crops compared to N dose 3.

Table 6-9 Overview of the inorganic fertilizer applications (kg N ha^{-1}) in 2009 along the N dose rate (1 to 4) during the crop rotation of cauliflower (2 applications, at the start and 7 weeks later) and leek (1 application 5 weeks after transplanting)

N dose	cauliflower1	cauliflower2	leek
1	30	43	40
2	80	35	80
3 (=reference)	130	25	100
4	180	18	140

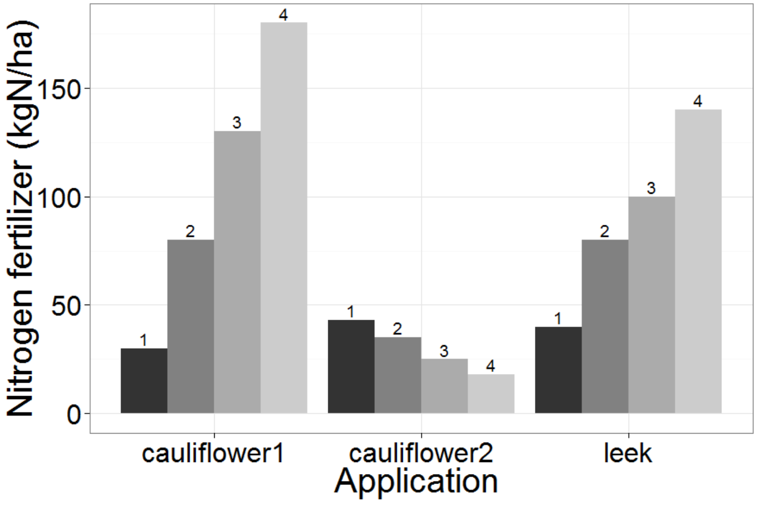

Figure 6-16 Overview of the inorganic fertilizer applications in 2009 along the N dose rate (1 to 4) during the crop rotation of cauliflower (2 applications, at the start and 7 weeks later) and leek (1 application 5 weeks after transplanting)

6.2.2 Model performance statistics

Similar to the calibration (see section 5.2) , the model performance was evaluated through both graphical techniques as quantitative statistics, including the time series plot of the constituent of interest, the plots of observed versus simulated output complemented by the set of statistical indicators, i.e. Nash-Sutcliffe efficiency (NSE), RMSE- observations standard deviation ratio (RSR) and percent bias (Pbias). The reliability of the model is thus tested for conditions outside the calibration environment as fertilizer rates differ.
Ultimate performance rating was achieved according to the same thresholds for calibration. Due to the different conditions as mentioned above, satisfying statistics (NSE > 0.5, RSR < 0.7 and Pbias<25%) would signify a good validation.

For the validation results an overview for all output is given in Table 6-10.

6.2.3 Validation output

The model output is in accordance with the calibration results and relates to the four main state variables concerning (1) the crop biomass including its nitrogen content, (2) the soil water content, (3) the soil temperature and (4) the soil nitrogen content. Their simulation was evaluated with the respective observations, as well as the unobserved processes which they interacted with.

6.2.3.1 Crop biomass and nitrogen uptake

Figure 6-17 shows the growth rotation cycle of cauliflower and leek in 2009 under four different N dose rates. The boxplots again represent the observed biomass production at each of the destructive sampling days. As confirmed by the performance ratings in Table 6-10 fair to even very good predictions were made of the crop dry matter growth as well as the nitrogen demand, for both cauliflower and leek, except for the lowest N dose rate at which the model underestimated the curd growth.

Regarding the highest N dose 4, predictions were similar to the reference as expected due to the lack of a negative ‘surplus’ factor. Nevertheless, it seemed still justified as observational differences between the two rates were not statistically significant (see Chapter 3).

Compared with the reference N dose 3, a total decrease of 56% and 24% in the respective lower N dose fertilizer applications 1 & 2 resulted in a shoot DM loss of 20% and 7% according to the observations, while simulations estimated the decrease at 33% and 13% respectively. Whereas leek yielded similar amounts under the different N dose rates, the model expected only a deficiency under N dose 1 decreasing the shoot DM yield by 9%.

Similar conclusions are valid for the respective plant organs yield. Simulations predicted for each a bigger decrease, on average by 7% up to 13% more than was measured. The biggest differences were found for the lowest N dose. To a certain extent the same results can be found regarding the nitrogen content which reflects the N demand and actual uptake (Figure 6-18). The model furthermore partitioned on average 5% more N towards the leaves than the fruit compared to the measurements regarding N dose 1 & 2 for both crops. For the leek crop, the shaft diameter and length was predicted similar under the different N dose rates as it only depended from ATT (Figure 6-19). As observations of the leek shaft dry matter did not differ much for the different rates, the simulated values regarding diameter almost all achieved a fair rating, while the length was rather underestimated. Statistically, no significant difference was found between two successive N dose rates, except for the lowest, regarding the observed fresh weight of the shaft nor its diameter or length. The difference in total fresh weight was caused by the difference in leaf fresh weight.

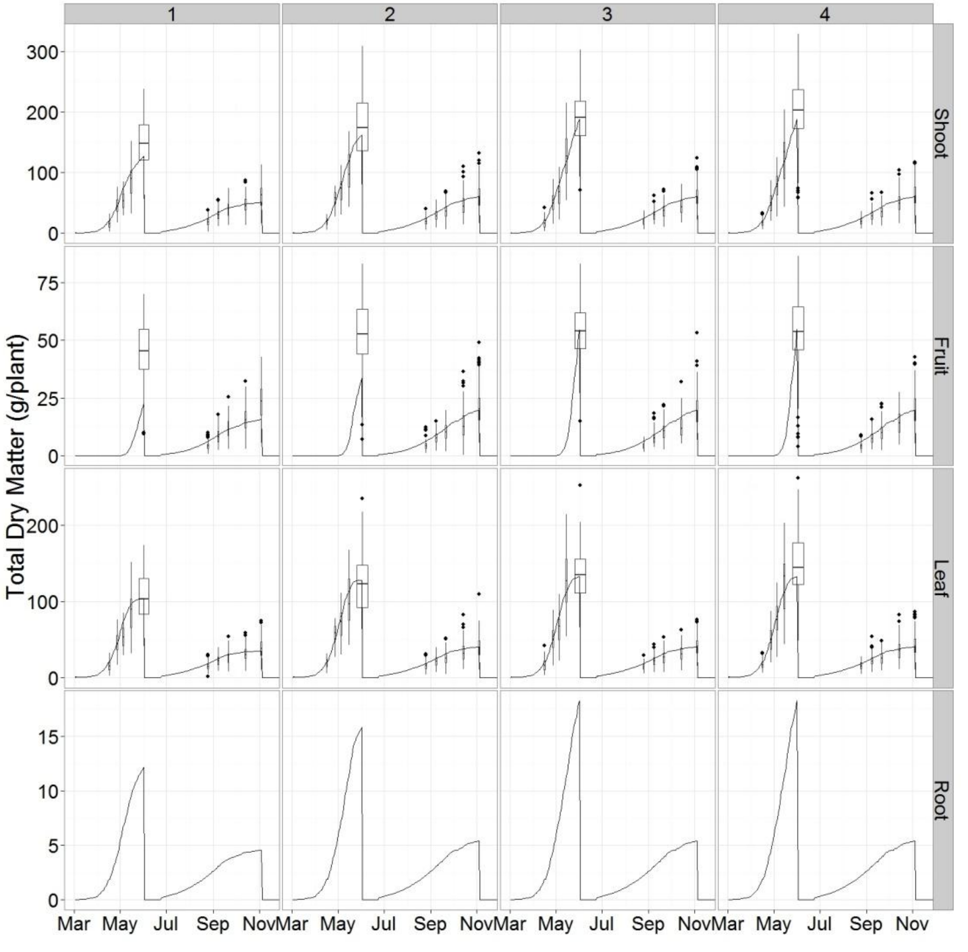

Figure 6-17 Validation output of the biomass or dry matter under the four different N dose rates for a rotation of cauliflower and leek, i.e. for the shoot, the fruit, the leaves (including the stem for cauliflower) and the roots. Boxplots denote the measurements (the box shows the 1st and 3rd quartile around the median, whiskers are extended to values within the 1.5*box length or 1.5*interquartile range; outliers are shown by black dots) and simulated growth is presented by the solid line.

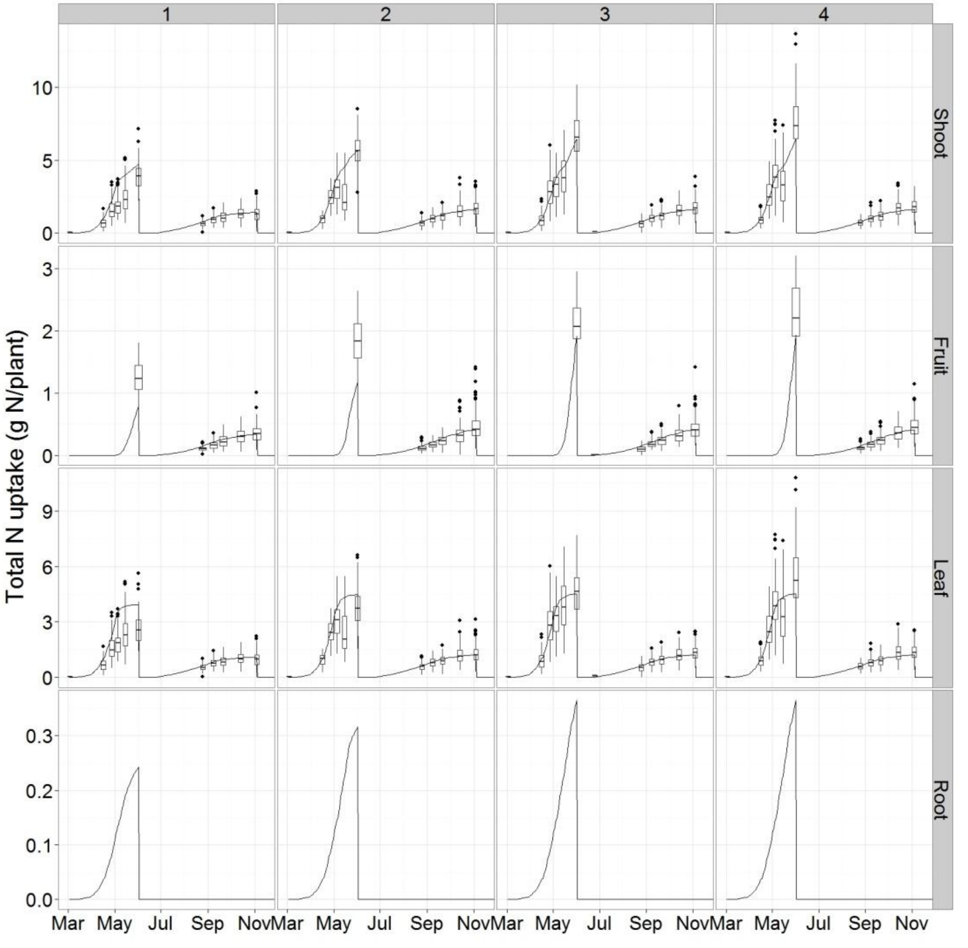

Figure 6-18 Validation output of the N uptake under four different N dose rates for cauliflower and leek, i.e. for the shoot, the fruit, the leaves (including the stem for cauliflower) and the roots. Boxplots denote the measurements (the box shows the 1st and 3rd quartile around the median, whiskers are extended to values within the 1.5*box length or 1.5*interquartile range; outliers are shown by black dots) and simulated N demand is presented by the solid line.

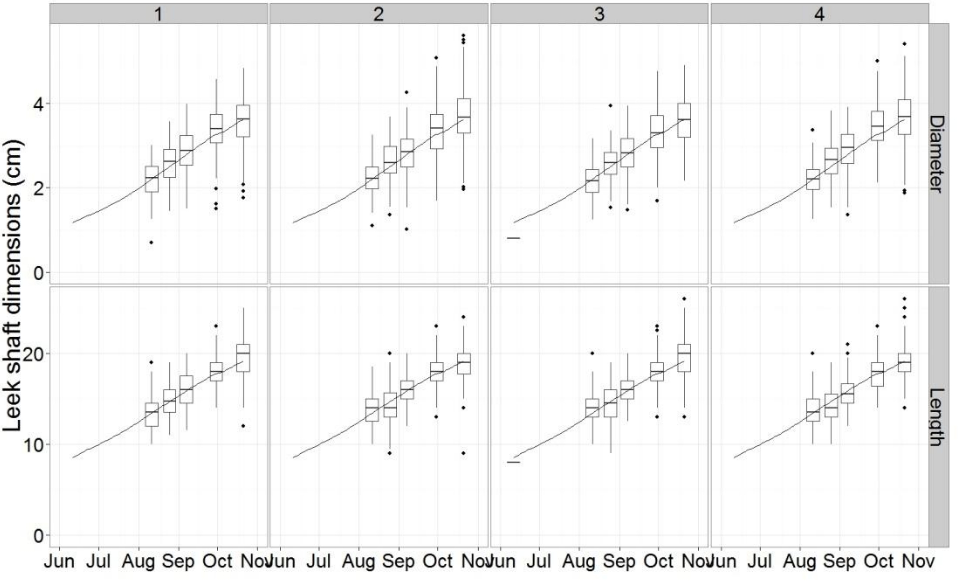

Figure 6-19 Validation of the leeks shaft properties, i.e. the diameter and length under four different N dose rates. Boxplots denote the measurements (the box shows the 1st and 3rd quartile around the median, whiskers are extended to values within the 1.5*box length or 1.5*interquartile range; outliers are shown by black dots) and simulation is presented by the solid line.

As with calibration, the approximation of the model predictions with the observations was quantified by the performance statistics as mentioned above and shown in Table 6-10. Overall fair to even very good ratings for NSE, RSR and Pbias were achieved for the crop growth under the different N dose rates.. Poor results were obtained for the Fruit dry matter under N dose 1 due to an underestimation, while the N content in the corresponding leaves were overestimated. Although close to the thresholds, poor ratings were found for the shaft properties of the leek, especially the length under the lower N dose rates.

Table 6-10 Overview of validation output for the four different N dose rates with model performance statistics (bold, regular and *(*) values indicate respectively a rating of poorly, satisfactory and (very) good).

		$\overline{O_i}$	sd_{O_i}	S_h	NSE	RSR	Pbias
	N dose	Cauliflower Leek		at harvest	whole rotation cycle		
Dry matter (g DM plant^{-1})							
Shoot	1	150.9	38.7	126.6	0.72*	0.53*	-2.16**
		62.3	18.8	51.1			
	2	175.7	51.1	162.0	0.76**	0.49**	4.45**
		60.8	19.0	60.0			
	3	188.1	42.6	187.9	0.83**	0.42**	5.73**
		60.9	17.3	60.0			
	4	204.9	56.5	187.9	0.79**	0.45**	2.78**
		62.7	19.8	60.0			
Fruit	1	44.6	13.3	22.6	**0.29**	**0.84**	**-27.41**
		23.5	7.8	15.8			
	2	52.5	15.0	33.6	0.57	0.65	-8.89**
		20.6	7.6	19.7			
	3	53.6	12.0	54.9	0.78**	0.47**	6.16**
		19.7	6.8	19.7			
	4	53.4	15.3	55.0	0.69*	0.55*	8.97**
		19.9	6.9	19.7			
Leaf	1	106.5	29.6	104.0	0.73*	0.52*	6.16**
		38.6	12.0	35.3			
	2	123.3	41.9	128.4	0.73*	0.52*	7.35**
		40.1	13.0	40.4			
	3	134.6	34.8	132.9	0.80**	0.45**	4.77**
		41.2	11.5	40.4			
	4	151.6	47.0	132.9	0.77**	0.48**	-0.12**
		42.8	14.0	40.4			
Root	1	-	-	12.2	-	-	-
		-	-	4.6			
	2	-	-	15.8	-	-	-
		-	-	5.4			
	3	-	-	18.3	-	-	-
		-	-	5.4			
	4	-	-	18.3	-	-	-
		-	-	5.4			

Table 6-10 (Continued) Overview of validation output for the four different N dose rates with model performance statistics (bold, regular and *(*) values indicate respectively a rating of poorly, satisfactory and (very) good).

	N dose	$\overline{O_i}$	sd_{O_i}	S_h	NSE	RSR	Pbias
		Cauliflower Leek	at harvest		whole rotation cycle		
Nitrogen content (g N plant^{-1})							
Shoot	1	4.0	1.1	4.7	**-0.04**	**1.02**	**33.99**
		1.3	0.5	1.4			
	2	5.6	1.4	5.7	0.55	0.67	11.33*
		1.7	0.6	1.6			
	3	6.8	1.4	6.4	0.72*	0.53*	2.98**
		1.7	0.5	1.6			
	4	7.8	1.8	6.4	0.74*	0.51*	-2.00**
		1.8	0.6	1.6			
Fruit	1	1.3	0.3	0.8	0.65	0.59*	-4.76**
		0.3	0.1	0.3			
	2	1.8	0.5	1.2	0.67*	0.57*	-9.89**
		0.5	0.2	0.4			
	3	2.1	0.3	1.9	0.88**	0.35**	0.62**
		0.4	0.1	0.4			
	4	2.3	0.5	1.9	0.88**	0.35**	-7.42**
		0.5	0.2	0.4			
Leaf	1	2.7	0.9	3.9	**-0.23**	**1.11**	**37.67**
		0.9	0.4	1.1			
	2	3.8	1.2	4.5	**0.48**	**0.72**	14.02*
		1.2	0.4	1.2			
	3	4.7	1.2	4.5	0.72*	0.53*	2.14**
		1.3	0.4	1.2			
	4	5.6	1.6	4.5	0.69*	0.56*	-1.63**
		1.4	0.4	1.2			
Root	1	-	-	0.2	-	-	-
		-	-	-			
	2	-	-	0.3	-	-	-
		-	-	-			
	3	-	-	0.4	-	-	-
		-	-	-			
	4	-	-	0.4	-	-	-
		-	-	-			
Leek shaft (cm)							
Diameter	1	3.5	0.6	3.6	**0.49**	**0.72**	-0.48**
	2	3.7	0.7	3.6	**0.48**	**0.72**	-2.33**
	3	3.6	0.6	3.6	0.56	0.66	-0.23**
	4	3.7	0.6	3.6	0.50	0.70	-2.81**
Length	1	19.4	2.1	19.1	**0.31**	**0.83**	-2.06**
	2	18.8	2.1	19.1	**0.27**	**0.86**	0.30**
	3	19.5	2.1	19.1	0.57	0.65	-1.97**
	4	19.3	1.9	19.1	**0.38**	**0.79**	-2.73**

Additionally to the model performance statistics, the graphic representation in Figure 6-20 shows how well the data of observations versus simulations fit the 1:1 line.

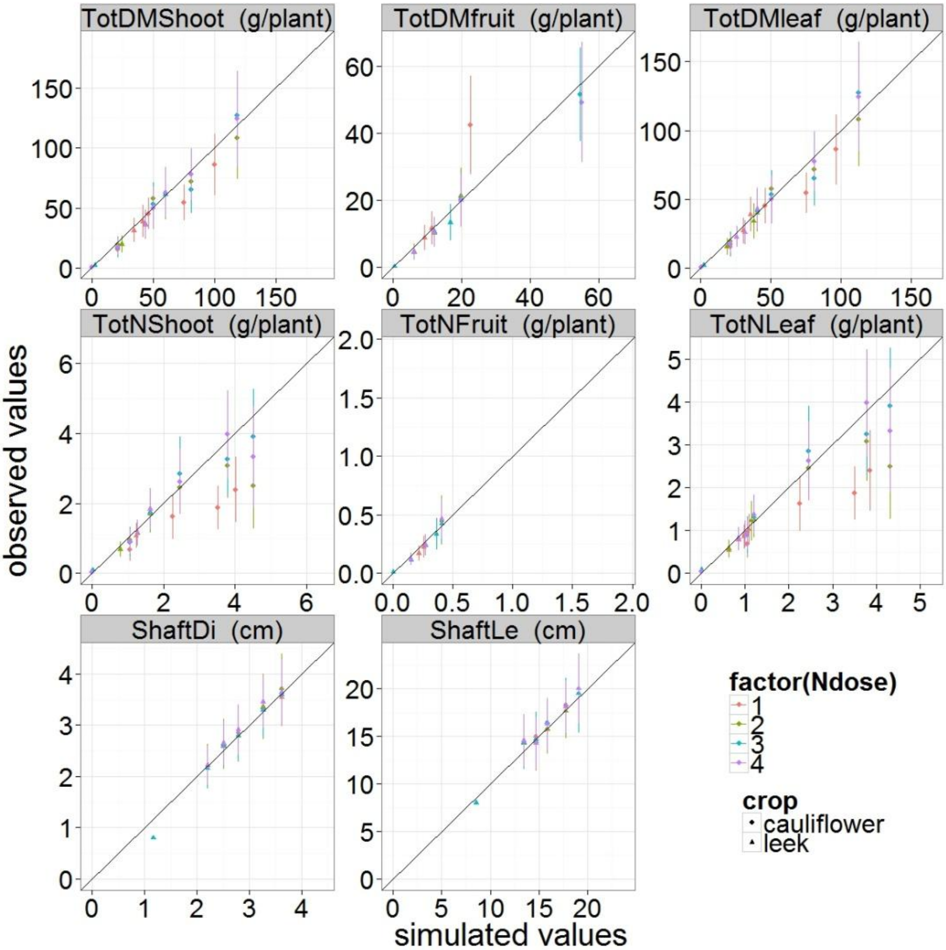

Figure 6-20 Overview of the model performance showing the observed versus simulated crop growth for the four different N dose rates regarding crop dry matter (*TotDM*) and nitrogen content (*TotN***) for *shoot, fruit* and *leaf* for both cauliflower and leek; as well as stem or shaft properties, i.e. the diameter (*ShaftDi*) and length (*ShaftLe*) of the leek crop. Error bars denote the range of observed values around the average.**

6.2.3.2 Soil water content

The observed and simulated soil water content did not significantly differ under the different N dose rates. Only for the lowest dose the model predicted some changes regarding the soil water related flows (see further). In accordance with the calibrated reference N dose rate, no soil water stress occurred for the simulations under the other N dose applications.

6.2.3.3 Soil temperature

Since both soil cover and soil water content hardly differed between the N dose treatments, also the soil temperature, observed as well as predicted, did not show significant differences between the different rate applications.

6.2.3.4 Soil mineral nitrogen content

Simulation of the soil nitrogen content in two consecutive soil layers of 30 cm, similar to the soil water content, was validated with the observations in the fields under different N dose rates in 2009.

Although the performance ratings in Table 6-11 do not represent a (very) good nor fair simulation according to the strict predefined thresholds, the model does seem to approach the overall trend of the soil nitrogen content during the rotation cycle under the different N dose rates as shown in Figure 6-21. The limited number of replications and samples taken over time and the high sampling error made verification of the models accuracy very difficult over the whole simulation period very difficult.

As the fertilizer N dose decreased to the lower rates, the soil nitrogen content, ammonium as well as nitrate, reached minimum levels unavailable to be taken up, creating an N stress for the crop. Compared to nitrate, the ammonium remains relatively constant as inputs from fertilizer and mineralisation are mostly nitrified very fast or emitted as ammonia. The differences in content after different N dose applications is thereby cancelled at the moment of harvest, with exception of the highest N dose rate for cauliflower and the lowest for leek respectively. Due to the fertilizer applications, the soil nitrate content stays elevated over the crop periods corresponding with the difference in N dose rates. Along the fallow period, the soil mineral nitrogen contents converge towards similar levels. Considering the good model performance to predict crop growth and soil water content, further refinement of the parameters regarding soil N processes, especially the influence of temperature and moisture, is required. After the cauliflower harvest, during summer, the model overestimates the ammonium content and underestimates the nitrate content in the upper 30 cm due to a high mineralisation and/or low nitrification. In the soil layer below, the model underestimates the ammonium content while the observed nitrate content is fairly approached which rather suggests more buffer through adsorption might be in order. On the other hand, further tweaking of the vertical distribution of nitrogen in the soil profile regarding percolation, gradient flow and/or the root depth and the distribution of uptake along that depth, could enhance the model performance.

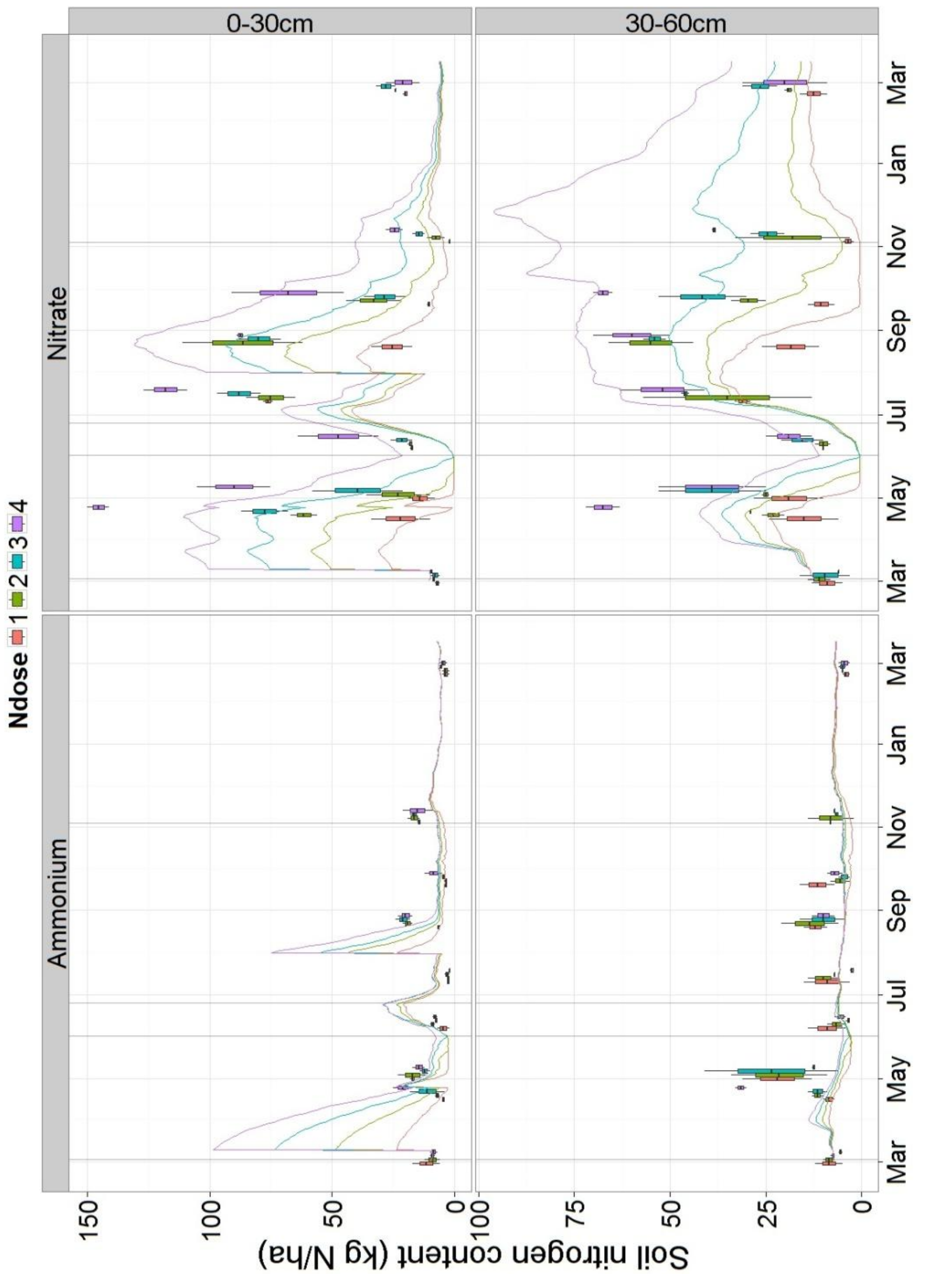

Figure 6-21 Validation of soil nitrogen content as nitrate and ammonium (in kgN ha^{-1}) in soil layers 0-30cm (upper) and 30-60cm (lower) for the four different N dose rates with observed values represented by the boxplots the box shows the 1st and 3rd quartile around the median, whiskers are extended to values within the 1.5*box length or 1.5*interquartile range; outliers are shown by black dots) and simulated contents presented by the solid line. Vertical dashed lines represent the growing periods of cauliflower and leek.

Table 6-11 Validation of soil nitrogen content (for ammonium and nitrate separately) in two consecutive soil layers of 30cm for the four different N dose rates with respective model performance statistics (bold, regular and *(*) values indicate respectively a rating of poorly, satisfactory and (very) good)).

	N dose	$\overline{O_i}$	sd_{O_i}	$\overline{S_i}$	NSE	RSR	Pbias
Soil ammonium content (kg N ha^{-1})							
0-30cm	1	7.6	5.7	6.6	**-0.62**	**1.27**	-13.13*
	2	9.7	6.7	8.3	**-0.27**	**1.12**	-13.80*
	3	10.0	6.3	10.07	**-0.75**	**1.32**	0.70**
	4	11.3	7.2	11.9	**0.05**	**0.97**	4.86**
30-60cm	1	10.3	6.7	5.1	**-0.82**	**1.35**	**-50.16**
	2	10.0	7.6	5.7	**-0.36**	**1.17**	**-43.0**
	3	8.8	8.7	6.0	**-0.08**	**1.04**	**-32.12**
	4	9.5	8.6	6.3	**0.06**	**0.97**	**-34.21**
Soil nitrate content (kg N ha^{-1})							
0-30cm	1	21.6	21.8	10.7	**0.09**	**0.95**	**-50.28**
	2	37.4	30.6	21.8	**0.38**	**0.79**	**-41.89**
	3	42.8	31.1	35.6	0.55	0.67	-16.80
	4	67.9	46.7	57.1	**0.41**	**0.77**	-15.97
30-60cm	1	14.3	9.5	12.9	**-0.08**	**1.04**	-9.74**
	2	25.1	16.8	20.1	**0.38**	**0.79**	-19.61
	3	31.7	15.9	31.0	0.56	0.66	-2.13**
	4	41.1	23.4	48.4	**0.11**	**0.94**	17.79

6.2.3.5 Other soil processes

Model output under four different N dose rates regarding unobserved processes including the nitrogen emissions are presented in Figure 6-22 and Figure 6-23 similar to the flow output at calibration. An overview of the quantitative soil water and nitrogen flows is listed through the respective balance in Table 6-12 and Table 6-13.

Water flow

Only the fields with the lowest N dose, showed a small difference from the higher dose fields as listed in the balance in Table 6-12. Due to lower crop growth, 9% less water was intercepted and 1% more runoff was simulated. Furthermore, 2.8% shifted from plant transpiration to soil evaporation, due to lower water uptake. The latter also contributed to an increase of 4% of water leaching to the ground water table. Overall the net change in water content remained equal for the fields under different N dose rates.

Table 6-12 Simulated soil water balance during the 2009 rotation cycle validated under the four different N dose rates.

	N dose			
Water flow (cm)	**1**	**2**	**3**	**4**
Rain	+73.13	+73.13	+73.13	+73.13
Irrigation	+12.85	+12.85	+12.85	+12.85
Interception	-6.93	-7.62	-7.62	-7.62
Runoff	-10.21	-10.05	-10.06	-10.06
Net SWC_{tot} change	+1.84	+1.84	+1.84	+1.84
Soil evaporation	-20.58	-20.03	-20.02	-20.02
Plant transpiration (=water uptake)	-28.95	-29.77	-29.79	-29.79
Deep percolation	-21.15	-20.35	-20.33	-20.33
Balance	≈0	≈0	≈0	≈0

Nitrogen flow

The soil organic matter (SOM) pools mineralized cumulatively proportional with the N dose rate (Table 6-12), with a maximum decrease in June of 18% and 13% for the lower doses respectively compared to the reference. Under the highest N dose however, a decrease as well was simulated by 4% as relatively less crop residue from cauliflower was incorporated. Over the whole cycle, the decrease was limited to 8, 5 and 1% for N dose 1, 2 and 4 respectively.

Compared with the reference N dose 3, ammonia volatilisation showed proportional changes the decrease of 56% and 24% in the respective lower N dose applications and the increase by 32% for N dose 4 showed proportional changes in ammonia volatilisation. For the other emissions, the changes do not follow the same ratio. The model predicted 44% and 15% less nitrification for N dose 1 & 2 and 10% more for the highest N dose compared to the reference, which is extended to the NO_x and N_2O emissions. The latter is even more increased as an extra 5% denitrification is predicted in case of N dose 4. Of the nitrogen uptake by cauliflower and leek respectively the share of ammonium is increased from 22% and 7% under the highest N dose up to 42 and 21% under N dose 1. Furthermore, as water percolates deeper into the soil, nitrogen is leached out cumulating up to 45% and 57% under the lower N dose rates respectively compared to the 60.5 kg N ha^{-1} under N dose 3, while 72% more is leached under the highest N dose. Ultimately, the amounts of water percolated would have nitrogen concentrations which range for the respective N dose rates from 14.6, 14.9, 15.3 and 15.6 mg L^{-1} during the early cauliflower cultivation, up to 12.7, 17.4, 32.3 and 57.2 mg L^{-1} during the fallow periods.

Table 6-13 Simulated soil nitrogen balance during the 2009 rotation cycle validated under the four different N dose rates.

	N dose			
Nitrogen flow (kgN ha^{-1})	**1**	**2**	**3**	**4**
Organic fertilizer	+60.57	+74.34	+105.21	+97.97
Mineral fertilizer	+113	+195	+255	+338
Net N_{org} change	+307.22	+302.49	+289.87	+294.78
Net N_{min} change	+6.13	-1.3	-20.02	-54.02
N uptake	-456.52	-531.69	-564.15	-565.62
NH_3 volatilisation	-0.95	-1.62	-2.29	-3.09
NO_x (nitrif)	-0.72	-0.93	-1.09	-1.20
N_2O ((de)nitrif)	-0.94	-1.18	-1.42	-1.64
N_2	-0.36	-0.41	-0.62	-0.90
N Leaching	-27.42	-34.71	-60.49	-104.27
Balance	≈0	≈0	≈0	≈0

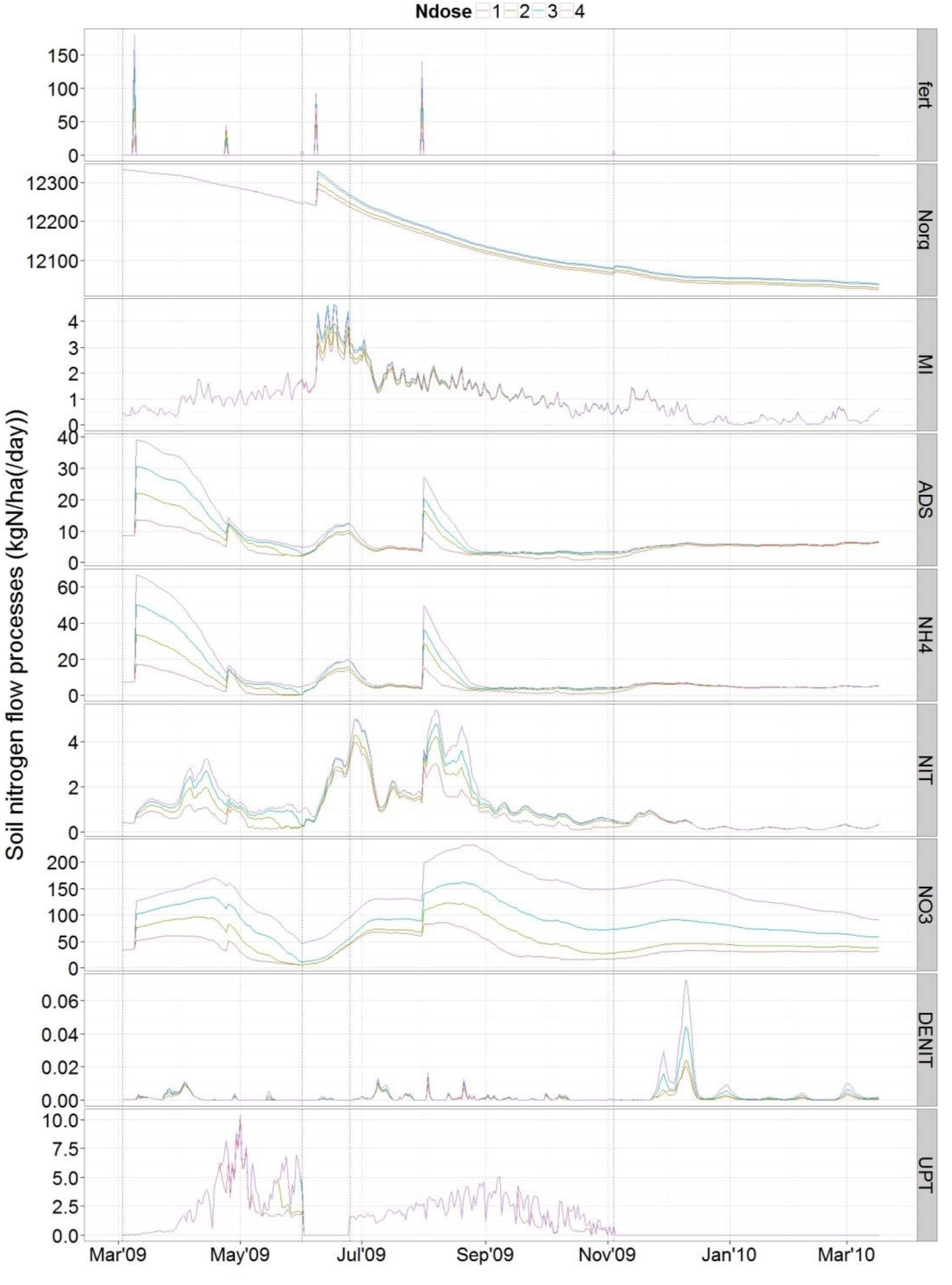

Figure 6-22 Overview of the simulated daily soil nitrogen flow processes (kgN ha^{-1} day^{-1}), i.e. fertilizer application (*fert*), mineralisation (*MI*), nitrification (*NIT*), denitrification (*DENIT*) and soil nitrogen uptake by crops (*UPT*), under four different N dose rates, affecting the total soil nitrogen contents (kgN ha^{-1}) of soil organic nitrogen (N_{org}), free (NH_4) and adsorbed (*ADS*) ammonium and nitrate (NO_3).

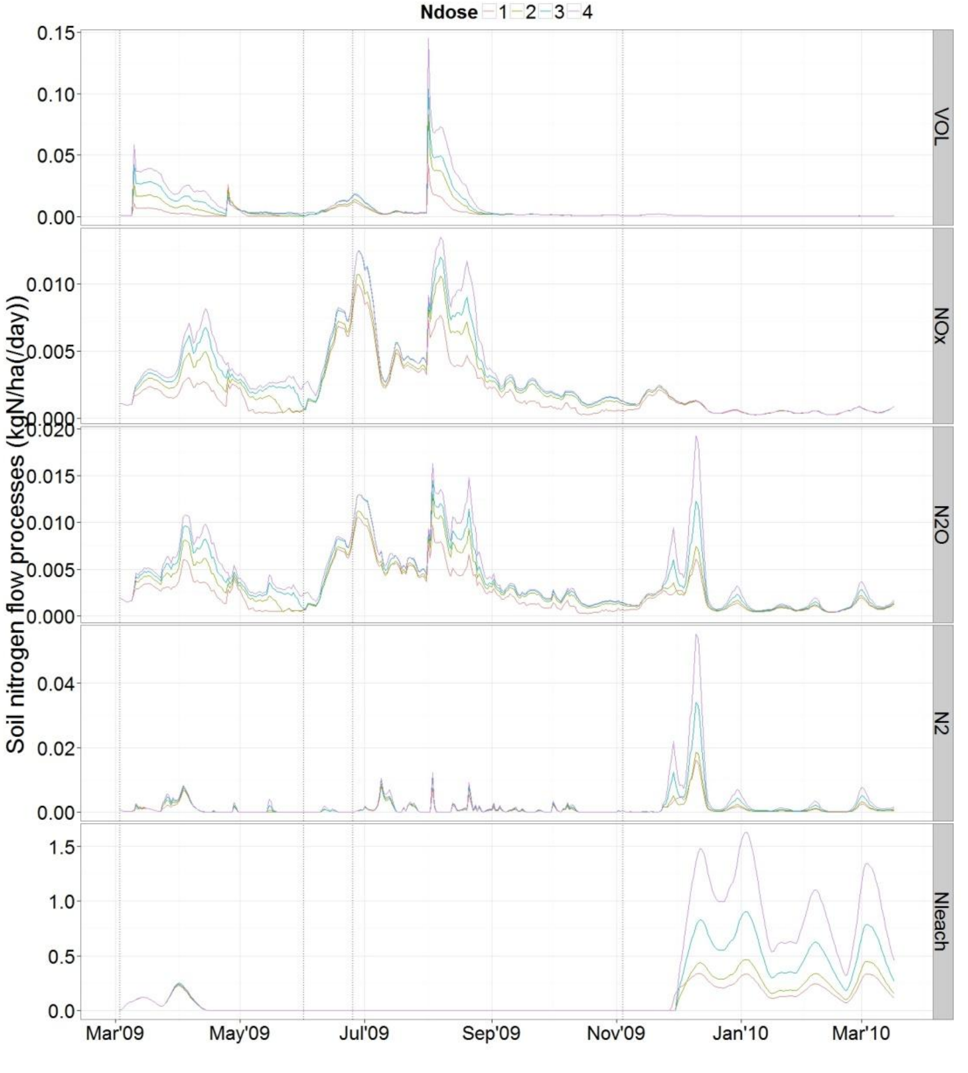

Figure 6-23 Overview of the soil nitrogen emissions (kgN ha^{-1} day^{-1}) affecting the total soil nitrogen content under 4 different N dose rates: ammonia volatilisation (*VOL*), nitrogen oxide (*NO_x*), dinitrogen oxide (*N_2O*), dinitrogen (*N_2*) and nitrogen leaching (*Nleach*).

Chapter 7. Model based Life cycle assessment

The main goal of this dissertation was to evaluate the environmental impact of a cauliflower-leek rotation. As discussed in Chapter 3 a life cycle assessment (LCA) was applied considering fertilizer production and application and the auxiliary equipment and energy use, based on the experiment as described in Chapter 2. Field emissions related to fertilizer application were estimated by commonly used empirical models. The mechanistic process oriented model (see Chapter 4) to simulate the nitrogen flow in a crop-soil system under given climate conditions, was however developed to provide an alternative approach to deal with the nitrogen dynamics. As the complex system of crop growth and soil processes features large variability under changing climate and different soil conditions the default LCA is expected to fall short due to its static nature and aggregated evaluation, especially when support is required for specific future management and its potential reduction of N emissions.

Therefore the LCA was rerun for the present case study with the model output (referred to by "model based LCA") and compared to the default LCA approach along with the respective assessment of the field emissions. Next, the model based approach was used in a scenario analysis which implies different reduction strategies accounting for the potential effects on crop yield and field nitrogen emissions.

7.1 Present case study

7.1.1 Goal & scope

The goal remained identical, but more relative, as a comparison was made of the environmental performance of a fertilizer management system towards sustainability increase according to the empirical and model based approach respectively. The response to four different nitrogen doses was assessed and more specifically the effect on the nitrogen field emissions, which contribute heavily to the LCA impact categories as already shown in Chapter 3.

System boundaries

Similar conditions and assumptions were made as with the empirical LCA (see section 3.1). To summarize, the LCA was limited from 'cradle-to-farm gate' and only included the fertilizer production, agricultural operations related to fertilizer application and corresponding construction, maintenance and disposal of infrastructure and auxiliary equipment to the extent of data availability in the databases queried.

The temporal boundary of each crop rotation system started at the planting date of cauliflower until the start of the next cauliflower crop, the year after, attributing all inputs and emissions to the rotation rather than the separate crops.

Functional unit
In order though to focus on comparing the field emissions and interpretation of the results from both approaches, the same yield, i.c. the simulated total dry matter of both crops (ton DM ha^{-1}), was used as functional unit (FU), while in Chapter 3 the fresh weight of the commercial yield was used. As addressed in the goal and scope, focus was put on the comparison and benefits of the model based approach rather than to assess the absolute impacts as such.

7.1.2 Life cycle inventory
The life cycle inventory (LCI) consists of the compilation and quantification of relevant inputs and outputs associated with the activities within the system boundaries and related to the production of the FU, including the use of resources and the emissions to air, water and soil. In this LCA study, on-farm emissions or foreground data related to specific agricultural inputs and practices were directly obtained from the experiment (e.g. fertilizer amounts) and estimated through either empirical models (default LCA) or the integrated model (model based LCA). Data associated with operations in the background system (e.g. fertilizer production) were taken from commonly accessed databases.

Foreground data
Retrieved data from the experiment with the applied N dose treatments is described in Chapter 2 and Chapter 3.

Field nitrogen emissions
For the model based LCA, field emissions of ammonia (NH_3), nitrate (NO_3) and nitrous and nitric oxide (N_2O and NO_x) to air and soil were estimated mechanistically (see sections 4.2 and 0) which differed from the empirical approach (see section 3.2). To summarize, ammonia is emitted according to a first order reaction from the ammonium pool which is fed by mineral fertilizers as well as mineralisation but also is decreased through nitrification. During the latter and subsequent denitrification of nitrate following a Michaelis-Menten function, NO_x and N_2O are released. Nitrogen is ultimately leached from the soil along with the soil water that percolates the different layers due to gravity. The model accounts for both ammonium and nitrate leaching (although ammonium has a very small share of 0.4-2%) while the empirical approach only considers nitrate to leach. All these processes are affected by the prevailing temperature and moisture conditions in the soil which change within and between the years of the rotation. Aggregated emissions are listed in Table 7-1, to allow a first evaluation and comparison in the assessment step.

Values might differ from the outcome of calibration and validation as small differences were implemented at the later stage of model implementation: i) crop residues of cauliflower were based on model output rather than the observed values and ii) the model simulation was run continuously from the start of 2009 until the cycle end of 2011 involving some issues of re-initialisation at the start of each rotation corresponding with the observations. Ultimately this aggregated into small differences in the water and nitrogen flow compared to the output of previous chapters. Nevertheless, this does not affect the general interpretation of the results comparing both approaches in the context of sustainability assessment.

Table 7-1 Overview of the simulated yield (cauliflower + leek, t DM ha^{-1}) and nitrogen emissions (kgN ha^{-1}) from the fields under different N dose rates.

	N dose	2009	2010	2011
yield (t DM/ ha)	1	14.2	9.8	6.1
	2	17.4	14.8	11.2
	3	18.4	18.7	16.6
	4	18.5	18.7	18.6
NH_3	1	0.94	0.52	0.21
	2	1.61	1.27	0.87
	3	2.26	2.19	1.80
	4	3.08	3.13	3.02
N_2O	1	0.92	0.79	0.58
	2	1.15	1.00	0.81
	3	1.39	1.49	1.18
	4	1.60	1.99	1.98
NO_x	1	0.71	0.46	0.31
	2	0.91	0.67	0.49
	3	1.07	0.95	0.70
	4	1.19	1.11	0.85
NO_3	1	26.6	32.5	21.8
	2	31.6	32.9	21.2
	3	59.5	76.5	33.1
	4	97.8	174.0	106.7

Background data

The LCA accounts for the emissions and processes related to fertilizer production and their application like fuel use and infrastructure. These general data as well as the characterisation factors, translating input data and field emissions into the environmental impact, were acquired from the life cycle inventory database Ecoinvent v2.2 (Frischknecht et al., 2005) corresponding with the LCIA methods mentioned beneath.

7.1.3 Life cycle impact assessment

The method of LCIA was performed in R according to CML2001 (Guinée et al., 2002) with the impact categories of acidification, global warming and eutrophication. The categories of human toxicity, cumulative energy demand and land occupation were excluded as the contribution of fertilizer application was zero to negligible as already stated in Chapter 3, thus their impact remained equal for both approaches. The same is valid for the components of fertilizer production and auxiliary material and energy for fertilizer application. Differences between both approaches can thus only be attributed to the difference in field emission estimation.

An overview of the environmental impact of the three rotation cycles in the consecutive years 2009-2011 is presented in Figure 7-1, corresponding to the four different N dose rates and the two approaches (default vs. model based). The results are expressed in each impact category relative to the functional unit, i.e. the total DM yield per ha. In Figure 7-2, these results are transformed to percentages, relative to the impact estimated by the empirical approach, as an extra perspective to facilitate the interpretation.
Overall, the impact associated with the mechanistic model based approach is consistently lower compared to the empirical results. Exceptions occurred regarding eutrophication for the higher N doses and, although less pronounced regarding global warming in 2011 under the lowest N dose. Generally, with increasing N dose application, did not only the impacts increase by 15% (except for NO_3 which depends of the year), but also the differences between both LCA approaches tend to increase from 21.5% to 34% for all impact categories, averaged over the years. Between the years, both approaches agreed for most on a higher impact during 2010, although not always as pronounced, while the year before and after, the impacts are more similar, especially for the higher N doses. The lowest N doses, especially in 2011, showed, also dependency on the approach taken.

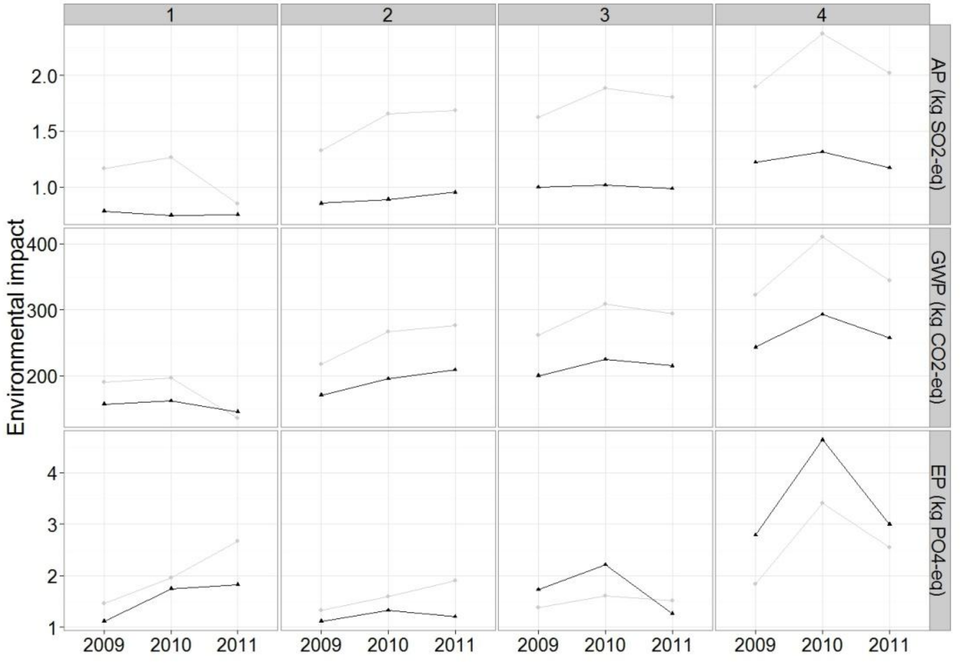

Figure 7-1 Environmental impact (acidification, AP; global warming, GWP and eutrophication, EP; in respective equivalents per functional unit of dry matter yield) as estimated by the default empirical (grey) and the model based (black) LCA regarding the rotation cycle in three consecutive years 2009-2011 under four N dose treatments (1-4)

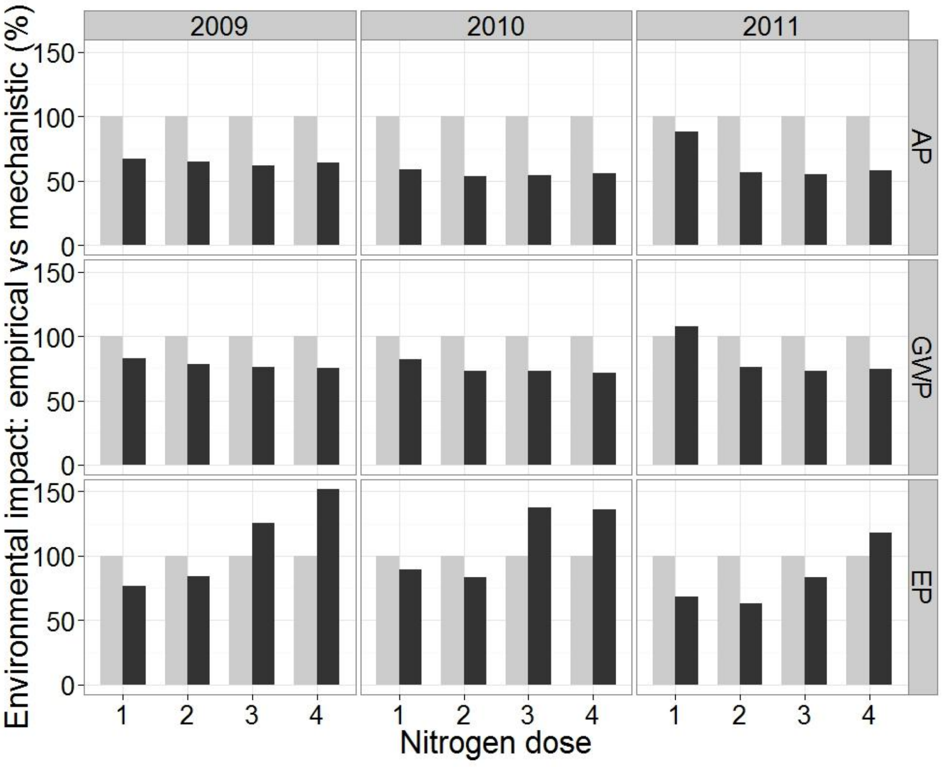

Figure 7-2 Relative environmental impact (acidification, AP; global warming, GWP and eutrophication, EP) as estimated by the empirical default (grey, 100%) and mechanistic model based (black) LCA regarding the rotation cycle in three consecutive years 2009-2011 under four N dose treatments.

Furthermore, the nitrogen emissions from the fields under the different N dose treatments are shown in Figure 7-3. The aggregated outcome of the default LCA approach are for visual reasons either attributed to the time of fertilizer application regarding ammonia emissions or distributed equally from monthly (nitrate leaching) or yearly (nitrous and nitric oxide emissions) values to daily values. To correspond with the LCA output from above, also the cumulative emissions per year are presented in Figure 7-4. Overall, the empirical approach generates a re-occurring pattern each year in the environmental profile, as fertilizer application management remained consistent and default monthly mineralisation is assumed along with the similar cultivation periods. Basically, this is also valid for the model based approach as the cumulative visualisation confirms, but is less clear because of the daily varying emissions.

As mentioned above, the differences between both approach estimations tended to increase with increasing N dose application regarding the impact categories. That is however not as straightforward for the field emissions. Whereas it might be valid for NH_3 and N_2O emissions, it is the opposite for NO_x and variable for NO_3. The model based NH_3 and N_2O emissions reaches on average only 77% and 61% of the empirically estimated values, while NO_x is emitted by almost twice the amount estimated by the empirical approach. Regarding NO_3 leaching, the cumulative impact according to the model based approach becomes higher than the empirically estimated values with increasing N dose treatment. Compared to the other impact categories, the NO_3 leaching is much less affected by the N dose application according to the empirical estimation. Furthermore, between the years differences in emissions dependent from the approach taken and N dose applied. Whereas emissions during 2010 are higher than the other years according to the empirical estimation, this is not reflected by the model based outcome, in particular for NH_3 and N_2O under the higher N doses or the lower ones regarding nitrate leaching.

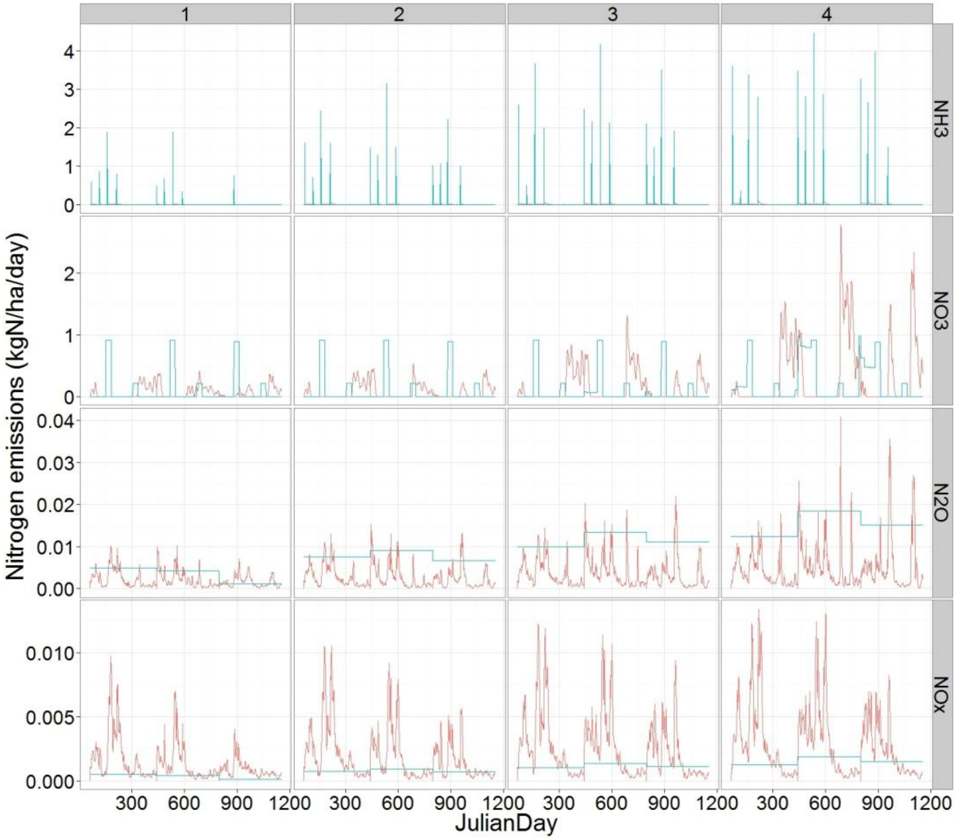

Figure 7-3 Field nitrogen emissions (ammonia volatilisation, NH_3; nitrate leaching, NO_3, nitrous and nitric oxide emissions (N_2O and NO_x) during the consecutive years of 2009-2011 under the different N dose (1-4) fertilizer applications, estimated by the empirical (blue; monthly (NO_3) and yearly (N_2O & NO_x) values are divided by the respective amount of days) and model based (red) LCA approach.

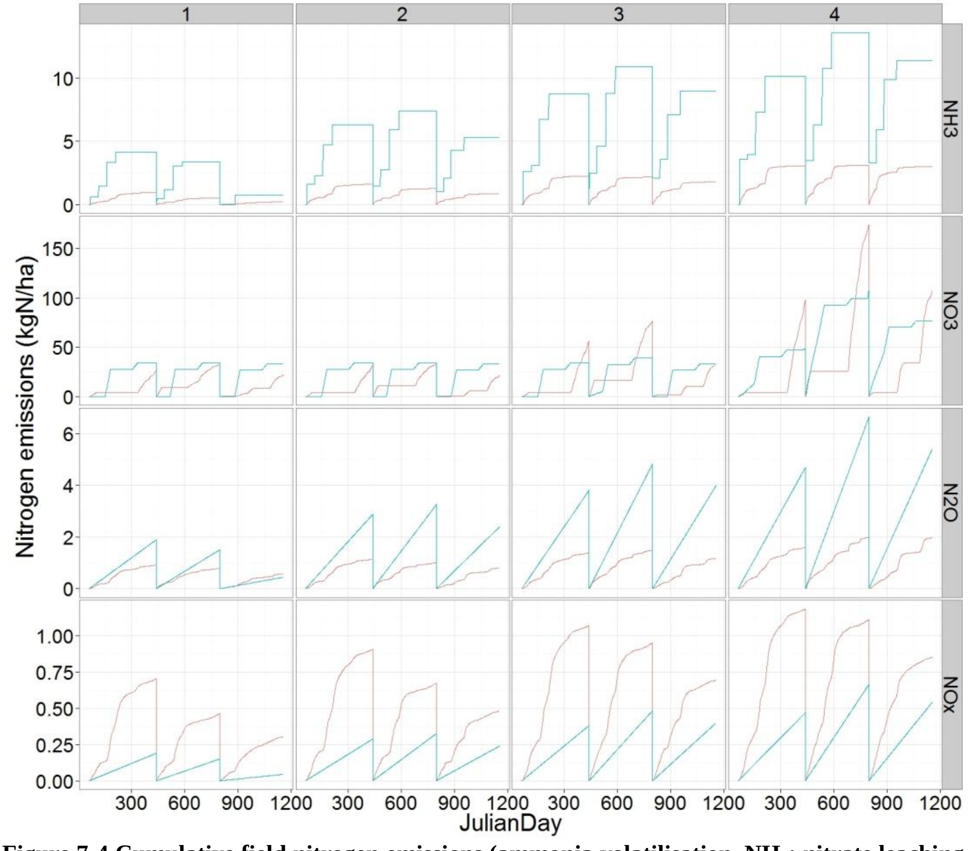

Figure 7-4 Cumulative field nitrogen emissions (ammonia volatilisation, NH_3; nitrate leaching, NO_3, nitrous and nitric oxide emissions (N_2O and NO_x) for every year under the different N dose (1-4) fertilizer applications, estimated by the empirical (blue) and model based (red) LCA approach.

7.1.4 Interpretation

Based on the first LCA results, a reduction in fertilizer input reduced the impact in all categories, the land occupation let aside. However, as results are expressed relative to the yield, a reduction in fertilizer input does not necessarily reduce the environmental impact (per unit DM produced), e.g. when low yields occur due to unfavourable conditions as the specific case in 2011 for N dose 1 shows. Generally the impact reduction according to the model based approach is less than estimated by the empirical approach, although still significantly as such. The model integrates after all multiple processes that interact on the soil ammonium and nitrate which are supplied with fertilizers and mineralisation processes, whereas the latter are directly linked to the emissions according to the empirical approach. Moreover, the different pathways of volatilisation or nitrification are affected by soil conditions as temperature and moisture, which are not accounted for by the empirical estimations.

Let aside the reduction of impact that could be achieved by introducing more sustainable technologies to produce the fertilizers and auxiliary equipment, both LCA outcomes require further and more detailed analysis of the underlying field emissions in order to suggest potential strategies. In a dynamic system like the water and nitrogen flow in a crop-soil system, impact assessment should address 'when' even more than 'which' potential reduction strategies should be implemented.

Potential reduction strategies:

- *Regarding ammonia volatilisation*: the empirical approach directly links NH_3 to the applied fertilizer. Considering for instance fractionated application of the N dose would not reduce the aggregated emissions and therefore also not its corresponding acidification and eutrophication potential impact. This option could however have implications in reality according to the implemented model as part of the fertilizer will follow alternative pathways depending on the prevailing weather conditions. It might be transported to lower soil layers with the gravitational water due to precipitation and/or nitrification transforms the ammonium into nitrate which favours the crop uptake or on his turn its potential leaching. Depending on the soil conditions and crop growth, multiple processes compete for the available ammonium which might lower the potential volatilisation. This interaction requests a model based approach.
- *Regarding nitrate leaching*: Figure 7-3 shows completely different periods when NO_3 is leached to the ground water table. The SALCA model applied by the empirical approach consistently assumes leaching in June during the fallow period between cauliflower and leek. The monthly time step however could have created this potential artefact, as this month does include mineralisation and crop residue incorporation but also leek transplants that take up nitrogen, although in small amounts. It was not clear how this approach deals with such discrepancy, as the primary cause of potential leaching, precipitation surplus, is not expected, unless long periods of rain would occur in that month. Whether or not the precipitation exceeds the evapotranspiration and/or nitrate from mineralisation/nitrification is still available for the following crop uptake can hardly be evaluated by the empirical approach, while a dynamic assessment could support the management to anticipate potential leaching. Assumed leaching in November, after leek harvest, is expected to occur later according to the integrated model, depending of the year and N dose treatment. The latter also predicts a cumulative increase in the fallow months until the new planted cauliflower reaches a significant uptake. As precipitation is not accounted for in the empirical approach, potential prevention of water infiltration during winter for instance would not affect the impact calculated by the empirical approach, while the model based estimation might suggest otherwise.

- *Regarding nitrous and nitric oxide emissions*: aggregated values from the empirical estimation do not allow much flexibility in the search for potential reduction strategies. The impact of ammonia volatilisations and nitrate leaching is linearly proportional to the applied fertilizer, thus it comes down to strategies as addressed above. With the current state of knowledge, the model based approach relates the emissions to the ammonium and nitrate pools with influence of temperature and moisture conditions. N_2O and NO_x are a by-product of nitrification of ammonia that is supplied by mineralisation and inorganic fertilizers. N_2O emissions increase extra under denitrifying conditions when soil water content is high, which is also reflected by the nitrate leaching. It should therefore be a matter of i) controlling nitrification without jeopardizing the amounts of nitrate to meet the crop uptake demand and ii) prevent conditions that favours denitrification, although the latter might increase nitrate amounts that could percolate till a certain extent.

Again, the complex integrated system combining crop growth and soil dynamics, confirms the difficulties to present unambiguous reduction strategies. The empirical approach might look straightforward regarding alternative solutions, but it is limited and potentially ineffective. Differences between both approaches are expected to stand especially when potential reduction strategies or climate change might affect the crop-soil N dynamics. Moreover, the empirical approach lacks crop growth prediction for future scenario analysis, which in turn would influence their LCA results as it is the functional unit to which the output is normalised.

7.2 Scenario analysis

Well calibrated and validated models allow for efficient and extensive scenario analysis. Moreover they contribute to the understanding of interactions between environmental and management factors, facilitate long-term assessments with historical data and enable future scenario analysis. All this makes the full model a suitable tool to assess responses of the crop-soil system to, among others, different reduction strategies. As a kick-off for future implementation of the developed model, two potential reduction strategies and their combination were assessed to limit field nitrogen emissions in order to reduce the corresponding environmental impact, regardless of the immediate feasibility of this strategy.

7.2.1 Objective

According to the model based approach, the responses of a cauliflower-leek rotation system under three potential reduction strategies were compared with the reference conditions as addressed previously. More specifically, the effect on crop yield and field nitrogen emissions was assessed under the different N dose rates and consequently on the corresponding environmental impact.

7.2.2 Potential reduction strategies

The reference system (ref) includes the N dose rates and climate as observed and addressed under section 7.1. The potential reduction strategies were threefold:

1. *FF*: a fractionated (by 4) weekly fertilizer application of each N dose rate (with cumulatively the same amount): see Figure 7-5 regarding the reference N dose 3.
2. *SC*: a soil cover or plastic mulch during winter fallow period preventing water infiltration between the harvest of leek and the start of cauliflower of the next rotation cycle. This was implemented as if no precipitation occurred that period: see Figure 7-6.
3. *FFSC*: a combination of the two reduction strategies above

Applying the fertilizer at different times, even at mature stage of crop growth, would require a more sophisticated application technology, but not unfeasible. Furthermore, farmers could apply plastic covers, similar to frost protection, which prevent the precipitation from infiltrating and would direct the runoff water straight to the drainage system, most of the time present in intensive horticulture.

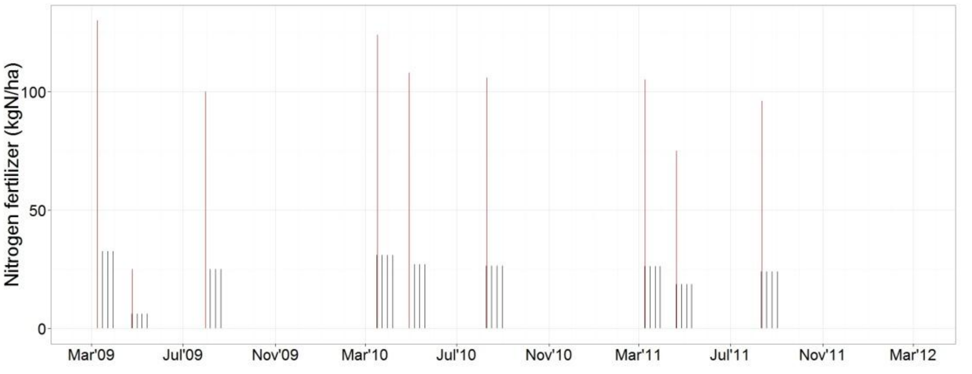

Figure 7-5 Overview of the fertilizer application scheme (i.c. N dose 3) according to the reference (red) and the fractionated alternative (black): every year of 2009-2011, each N dose rate (2 times for cauliflower, one time for leek) is divided by 4 in a weekly application

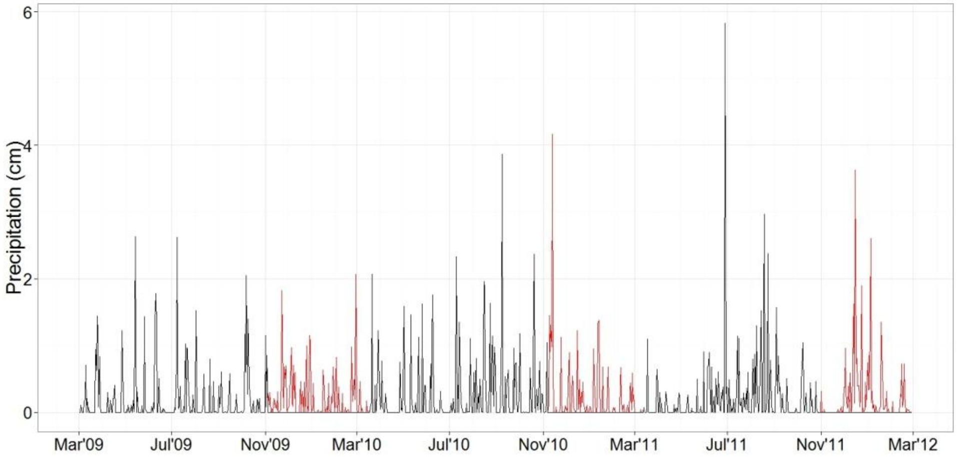

Figure 7-6 Overview of the precipitation during 2009-2011 according to the reference and the potential reduction strategies: in the latter, the amount during winter fallow periods (red) is prevented from infiltrating into the soil

7.2.3 Results

7.2.3.1 Crop yield

A quantitative overview of the scenario analysis output regarding crop yield is listed in Table 7-2. Figure 7-7 shows the growth rotation cycles of cauliflower and leek from 2009 to 2011 regarding the reference and the potential reduction strategy simulations.

Overall, the crops could have got more benefits from one or both the reduction strategies under the lower N dose rates compared to the higher and especially regarding cauliflower cultivation from March to June (see also bold values in Table 7-2). Looking at each crop cultivation each year, most of the times, under the lower N dose rates, yield would already benefit from a fractionated fertilizer application (FF and thus FFSC), which seems to correspond better with the daily N demand of the crop over its entire cultivation period. N stress is reduced, especially at the later stage of crop growth. In the two subsequent years 2010-2011, implementation of the soil cover (SC and thus FFSC) would overall further enhance the increase in yield. Under at least one of the reduction strategies, the increase of cauliflower yield could range from 0.4% up to 23% over the years for the two lower N dose rates, while leek would yield no more than 1.3% extra.

Under the higher N dose rates 3 and 4, only the soil cover strategy (SC) might be beneficial over the years depending on the conditions. Yield profits would be achieved of 1.7% for cauliflower in 2010, and 21.5% for leek in 2011 merely due to the build-up of nitrate content in the soil if a soil cover is applied in the winter fallow periods. It prevents the soil nitrogen of draining down which results in higher contents available for the crop over the whole cultivation period. In 2011 the wet summer/autumn decreased the potential leek yield under the reference system with N dose 3, while N dose 4 still provided enough nitrogen for the plant uptake.

Table 7-2 Overview of the simulated yield (cauliflower + leek, t DM/ha) in the years 2009-2011 from the fields under different N dose rates for the different strategy systems (FF: fractionated fertilizer application; SC: soil cover during winter fallow periods; FFSC: FF and SC combined) compared to the reference system (ref) with highest yields in bold.

N dose	Year	ref	FF	SC	FFSC
1	2009	14.14	**14.50**	14.13	14.50
	2010	9.78	10.07	10.20	**10.60**
	2011	6.10	6.10	**6.33**	6.30
2	2009	17.35	**17.37**	17.35	17.37
	2010	14.79	15.20	16.04	**16.20**
	2011	11.15	11.43	**11.96**	11.88
3	2009	18.41	**18.43**	18.41	18.43
	2010	18.66	18.66	**18.80**	18.80
	2011	16.59	16.59	**18.57**	18.57
4	2009	18.52	18.52	18.52	18.52
	2010	18.66	18.66	**18.80**	18.80
	2011	18.57	18.57	18.57	18.57

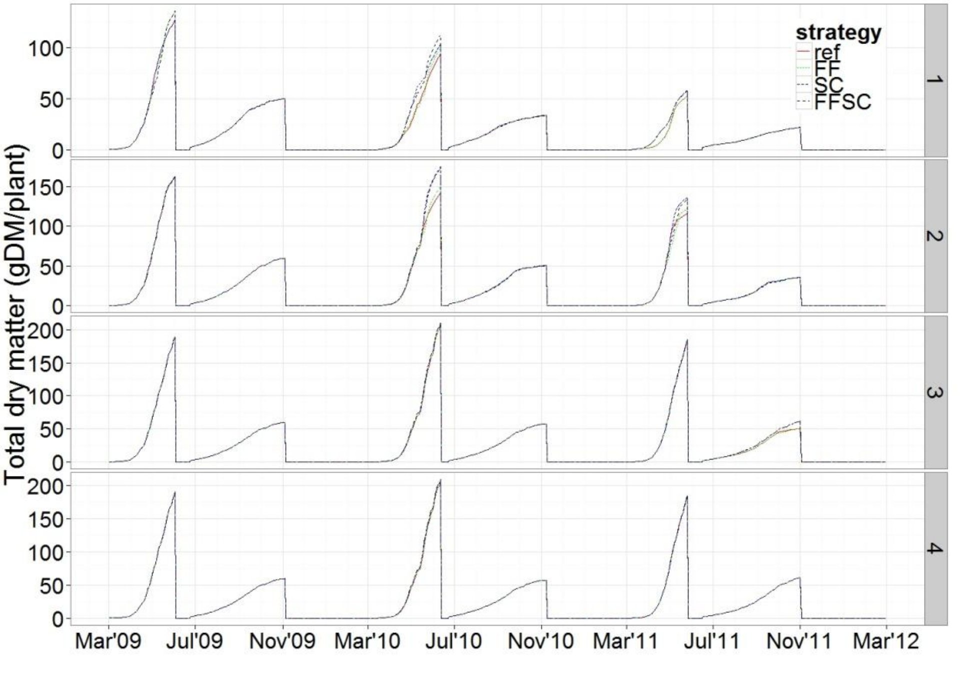

Figure 7-7 Cumulative crop growth of a cauliflower- leek rotation regarding the total dry matter during the consecutive years 2009-2011 under the different N dose rates 1-4 according to the reference (red) system and the potential reduction strategies with fractionated fertilizer application (FF, green), soil cover (SC, blue) and their combination (FFSC, black).

7.2.3.2 Field nitrogen emissions

A quantitative overview of the scenario analysis output regarding field nitrogen emissions listed in Table 7-3. Figure 7-8 show the daily release over the years under the different reduction strategy systems compared to the reference regarding N dose 3 (output of the other N rates are proportionally quite similar). A cumulative output is presented in Figure 7-9.

Overall, a reduction in field nitrogen emissions to the environment is expected implementing one or both the reduction strategies (with best results in bold in Table 7-3). Whereas the FF system benefits the environment regarding ammonia volatilisation (NH_3) and nitric oxide (NO_x) emissions, the SC system and even more the combined FFSC system reduces the nitrogen losses the most regarding nitrate leaching (NO_3) and nitrous oxide (N_2O) emissions. In some occasions an increase, although small, is simulated compared to the reference system (red values in Table 7-3). Furthermore, the extent of reduction is not related to the applied N dose rate.

Table 7-3 Overview of the nitrogen field emissions (kgN/ha) in the years 2009-2011 from the fields under different N dose rates for the different strategy systems (FF: fractionated fertilizer application; SC: soil cover during winter fallow periods; FFSC: FF and SC combined) compared to the reference system (ref) with lowest emissions in bold and higher emissions than the reference in red.

	N dose	Year	ref	FF	SC	FFSC
NH_3	1	2009	0.94	**0.84**	1.02	0.92
		2010	0.52	**0.45**	0.56	0.49
		2011	0.21	**0.21**	0.25	0.25
	2	2009	1.61	**1.35**	1.69	1.43
		2010	1.27	**1.04**	1.34	1.12
		2011	0.87	**0.68**	0.97	0.75
	3	2009	2.26	**1.98**	2.34	2.06
		2010	2.19	**1.93**	2.27	2.06
		2011	1.80	**1.44**	1.98	1.60
	4	2009	3.08	**2.73**	3.16	2.81
		2010	3.12	**2.94**	3.19	3.04
		2011	3.02	**2.36**	3.34	2.59
NO_3	1	2009	26.63	27.13	4.20	**4.17**
		2010	32.55	30.91	15.27	**14.60**
		2011	21.79	21.70	10.61	**10.10**
	2	2009	31.61	31.20	4.29	**4.22**
		2010	32.92	30.56	10.37	**9.86**
		2011	21.22	20.64	5.36	**5.24**
	3	2009	56.54	56.02	4.38	**4.26**
		2010	76.52	74.71	16.51	**15.70**
		2011	33.13	33.33	21.67	**20.54**
	4	2009	97.79	97.37	4.47	**4.31**
		2010	173.96	170.73	26.64	**25.50**
		2011	106.70	107.32	55.85	**54.32**
N_2O	1	2009	0.92	0.91	0.85	**0.84**
		2010	0.79	0.75	0.71	**0.68**
		2011	0.58	0.58	0.55	**0.54**
	2	2009	1.15	1.12	1.07	**1.04**
		2010	1.00	0.95	0.94	**0.90**
		2011	0.81	0.77	0.68	**0.64**
	3	2009	1.39	1.37	1.25	**1.23**
		2010	1.49	1.44	1.34	**1.31**
		2011	1.18	1.15	1.16	**1.14**
	4	2009	1.60	1.58	1.39	**1.37**
		2010	1.99	1.94	1.59	**1.55**
		2011	1.98	1.98	1.65	**1.64**
NO_x	1	2009	0.71	**0.70**	0.71	0.71
		2010	0.46	**0.45**	0.47	0.46
		2011	**0.31**	**0.31**	**0.31**	**0.31**
	2	2009	0.91	**0.89**	0.92	0.90
		2010	0.67	**0.65**	0.69	0.67
		2011	0.49	**0.47**	0.49	0.47
	3	2009	1.07	**1.06**	1.08	1.07
		2010	0.95	**0.94**	0.99	0.98
		2011	0.70	**0.69**	0.74	0.75
	4	2009	1.19	**1.18**	1.20	1.18
		2010	1.11	**1.10**	1.12	1.11
		2011	0.85	**0.85**	0.86	0.86

Ammonia volatilisation

Closely related to the fertilizer application, the peaks of ammonia volatilisation at the time of application during the reference management are reduced and spread over time along the fractionated application in the systems of FF and FFSC. From 5.8% up to 22% less ammonia emission is achieved in the different years under the different N dose rates regarding the FF scenario. Implementation of only the winter soil cover (SC) would however increase the ammonia loss with 2% up to 16% compared to the reference system due to relative higher soil ammonium contents in the upper layers during fallow periods as little to no drain occurs. Except for the year 2011 under N dose 1 (which lacks fertilizer addition), these extra losses are compensated in the FFSC scenario by the cumulative decrease in ammonia volatilisation. This might be related to the fractionated fertilizer application and the competition of multiple processes for the available ammonium as addressed in the model. Ultimately, this would lead yearly to 4.1%, 12.3%, 8.6% and 8.4% less ammonia volatilisation on average under the respective N dose rates.

Nitrogen leaching

Implementing a fractionation of the fertilizer application has no unambiguous effect on nitrogen leaching. Depending on the prevailing conditions a decrease of 7.2% up to an increase of 1.9% can be expected compared to the reference system. With the SC and FFSC system however, the lack of water infiltrating during the winter fallow periods prevents the soil water and nitrogen within from leaching to the ground water table. As the soil cover is removed at the start of the crop rotation, leaching still occurred during the early stages of cauliflower cultivation and during leek cultivation in 2011, due to a relative wet summer/autumn. With increasing N dose rate, the water uptake for plant transpiration increases, which results in a decrease of soil water percolation. The amount of dissolved nitrogen however increases with the application rate for all systems. Implementation of the winter soil cover would limit these nitrogen leaching losses each rotation cycle by 38% up to 95.6% compared to the reference system under the different N dose rates.

Nitrous oxide emissions

Whereas fractionation of the fertilizer application tends to decrease cumulative nitrification up to 3.7% compared to the reference system, it is not always the case regarding denitrification: from -10% to +2.5% looking at the different years and N dose rates. Again due to relative higher ammonium contents when winter soil covers are applied, more nitrification is predicted compared to the reference system. However, denitrification is then significantly reduced as the soil is not replenished by the precipitation during fallow periods, avoiding anaerobic conditions as they occur in the reference or FF system. Subsequently, yearly N_2O emissions are reduced from 0.2% up to 5.5% with the FF system and from 2.9% up to 21.8% if the soil cover is implemented as well under the FFSC scenario.

Nitric oxide emissions

Similar to the ammonia losses and related to the ammonium content, nitrification is slightly reduced under the FF system, but increased under the SC system. Consequently fractionated fertilizer application irrespective of the N dose, prevents 0.1% up to 3.7% NO_x to be emitted compared to the reference system, whereas 0.7% up to 3.6% more is lost under the SC system. Whereas one reduction strategy mostly supplements or positively compensates the other in the FFSC system, it is not always valid regarding NO_x emissions. Although the differences are small, implementation of the FFSC is expected to decrease NO_x yearly by 0.6% and 1.7% on average under N dose rate 1 & 2 respectively, it will however increase the yearly emission by 3.2 and 0.2% under respectively N dose rate 3 & 4.

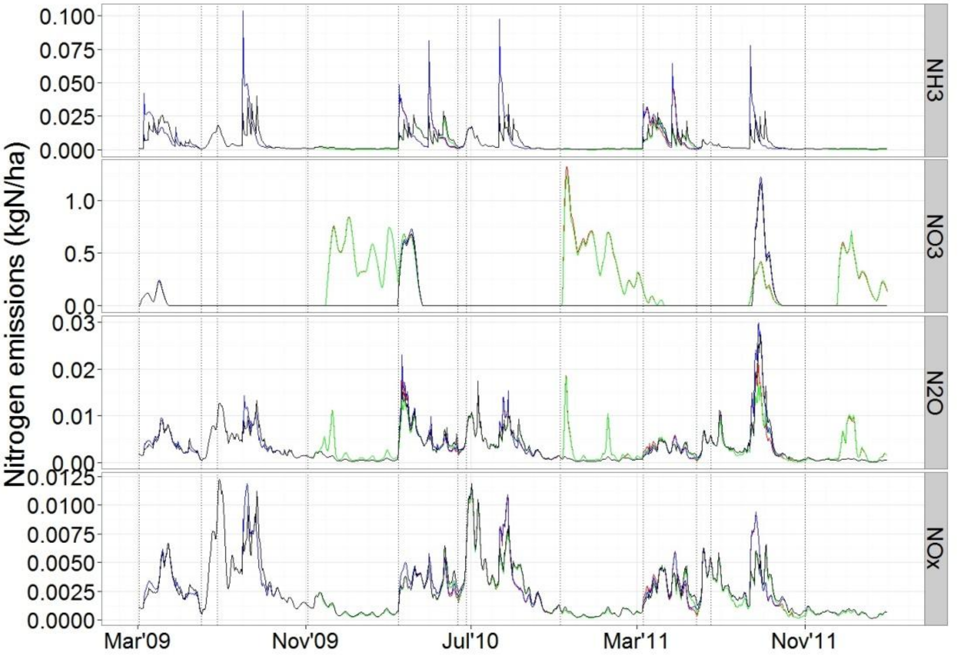

Figure 7-8 Soil nitrogen emissions during cauliflower- leek rotations in the years 2009-2011 regarding ammonia volatilisation (NH3), nitrogen leaching (NO3) and nitrous (N2O) and nitric (NOx) oxides, according to the reference (in red) and reduction strategy simulations (FF in green; SC in blue and FFSC in black) under the reference N dose 3 rate.

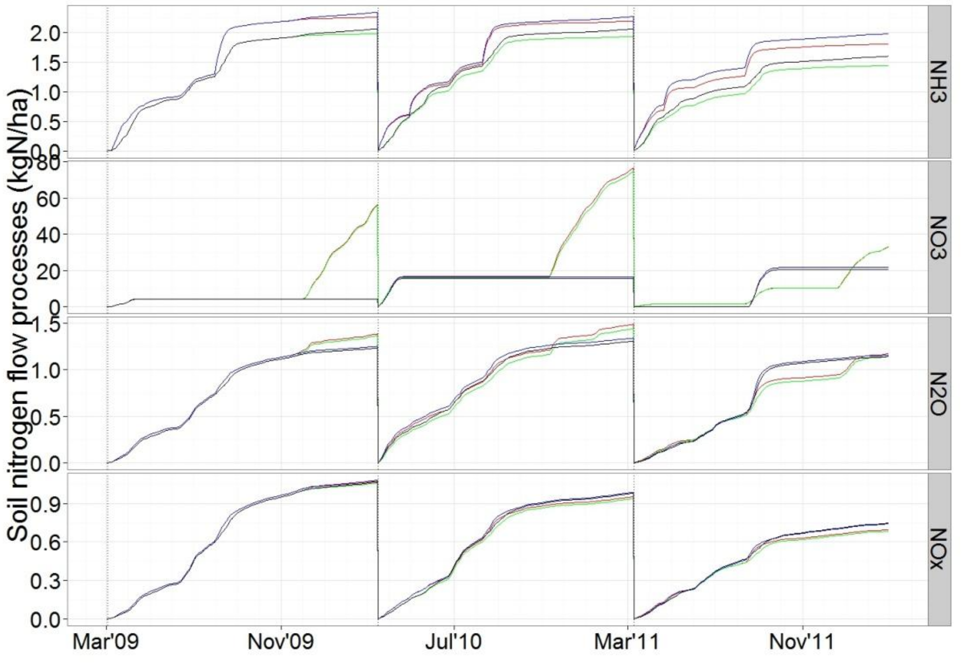

Figure 7-9 Yearly cumulative soil nitrogen emissions during cauliflower- leek rotations for the years 2009-2011 regarding ammonia volatilisation (NH3), nitrogen leaching (NO3) and nitrous (N2O) and nitric (NOx) oxides, according to the reference (in red) and reduction strategy simulations (FF in green; SC in blue and FFSC in black) under the reference N dose 3.

7.2.3.3 Life cycle assessment

Final step in comparing the scenarios involved a life cycle assessment quantifying the environmental burden of the different systems (FF, SC & FFSC) compared to the reference (ref), including the change of crop yield and nitrogen field emissions as addressed above.

Goal & scope

A comparison was made of the environmental impact of two different reduction strategies and their combination implementing fractionated fertilizer applications and winter soil covers for each crop rotation cycle under the different N dose rates, relative to the model based LCA as addressed in section 7.1.

The LCA was again limited to 'cradle-to-farm gate' and only included the fertilizer production, agricultural operations related to fertilizer application and corresponding construction, maintenance and disposal of infrastructure and auxiliary equipment to the extent of data availability in the databases queried. The temporal boundary of each crop rotation system started at the planting date of cauliflower until the start of the next cauliflower crop, the year after, attributing all inputs and emissions to the rotation rather than the separate crops.

The functional unit (FU) to which all input and output was normalized, was again the total dry matter of both crops (ton DM ha^{-1}) as predicted by the model under the different systems as listed in Table 7-2. As addressed above, focus was put on the comparison and benefits of the model based approach rather than to assess the absolute impacts as such.

Life cycle inventory

The life cycle inventory (LCI) was very similar to the previous model based LCA case study, with two main differences related to the reduction strategies:

1. Besides the on-farm emissions as predicted by the model, the yield as well differed between the scenarios.
2. The fractionated application of fertilizer (amounts as in the experiment, cf. Chapter 2 and Chapter 3) and implementation of plastic soil cover each winter fallow period was assumed to include additional materials and energy compared to the reference, accounting for the respective lifetime. Tractor use was increased for fractionated fertilizer application, while the soil cover implies the production of polyethylene sheets and its mulching process.

Data associated with operations in the background system (e.g. fertilizer production) were taken from commonly accessed databases as previously addressed.

Life cycle impact assessment

The method of LCIA was performed in R according to CML2001 and CED method with the impact categories of acidification, global warming, eutrophication, human toxicity, cumulative energy demand and land occupation.
An overview of the environmental impact of the three rotation cycles in the consecutive years 2009-2011 regarding the different reduction strategies is presented in Figure 7-10 corresponding to the four different N dose rates. The results are expressed in each impact category relative to the functional unit, i.e. the total DM yield per ha. In Figure 7-11, these results are transformed to percentages, relative to the impact of the reference system without fertilizer fractionation or winter soil cover.
Despite the potential yield increase, which corresponds with a lower land occupation (LO) up to 10.7% and a decrease of field nitrogen emissions, these benefits of a reduction strategy implementation are not reflected by the other LCA impact categories, except for the eutrophication potential. Whereas the fractionated fertilizer application system (2011 N dose 3 excluded) shows an increase of 1.1% to 14.9% in acidification, 9.5% to 20.3% in energy demand, 3.8% to 9.8% in global warming and 10.1% to 23.2% in human toxicity, the respective burdens over all years and N dose rates are even worse regarding the SC and FFSC system which include the plastic mulching during winter fallow periods. Both systems would raise the acidification by 67% to 220%, the energy demand by 376.2% to 917.5%, the global warming by 74.7% to 255.6% and human toxicity by 36% to 108.2%. Regarding the eutrophication however, the

effect of FF would range from -6.5% to +1.1% compared to the reference system, while winter soil cover implementation would decrease the impact category by 18.5% up to 73.9% depending of the year and N dose rate.

While the impact under the reference and FF system increases with increasing N dose rate, it is not the case for the SC and FFSC system. Implementation of the winter soil cover with the N dose 1 rate shows the highest impact (2[nd] highest regarding eutrophication), while with N dose 3 the impact is the smallest. Land occupation then again decreases with increasing N dose rate for all systems.

Between the three different years, the relative impact was similar for all systems, although a few exceptions occur regarding the eutrophication potential and the N dose 1 rate under the SC and FFSC system due to the wet summer/autumn in 2011 and the lack of fertilizer addition under N dose rate 1 in 2011.

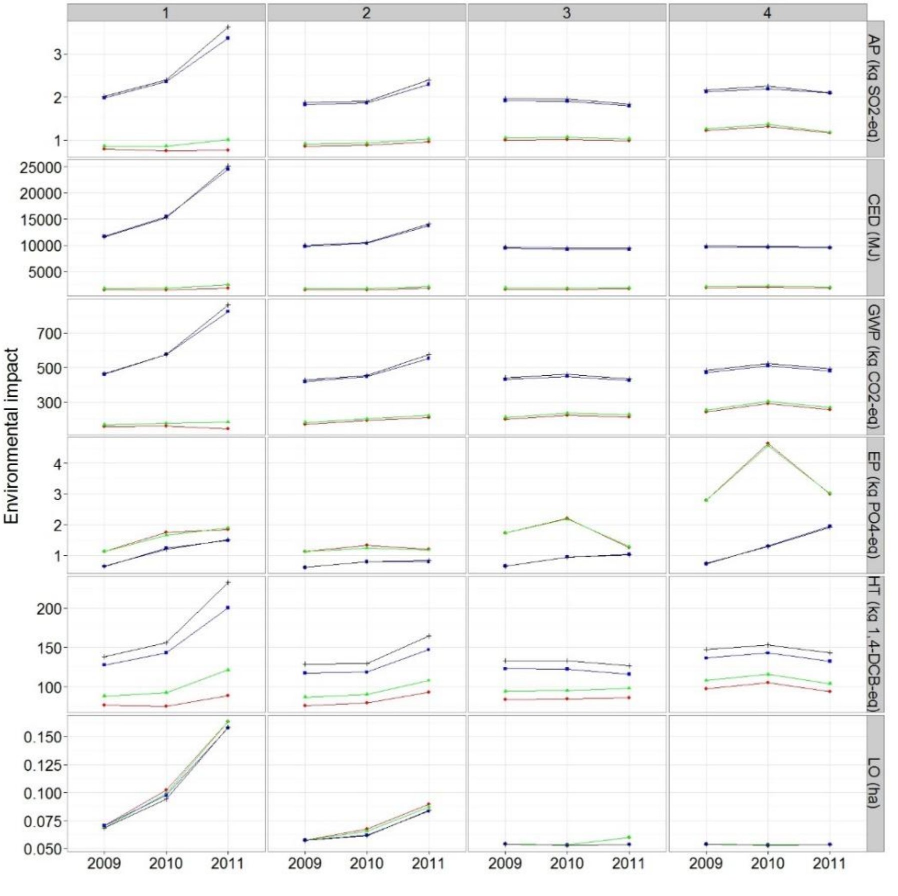

Figure 7-10 Environmental impact (acidification, AP; cumulative energy demand, CED; global warming, GWP; eutrophication, EP; human toxicity, HT and land occupation, LO, all in respective equivalents per functional unit of dry matter yield) as estimated by the model based LCA regarding the rotation cycle in three consecutive years 2009-2011 under the four N dose treatments (1-4) and according to reference system (in red) or the implemented reduction strategies (FF in green, SC in blue and FFSC in black))

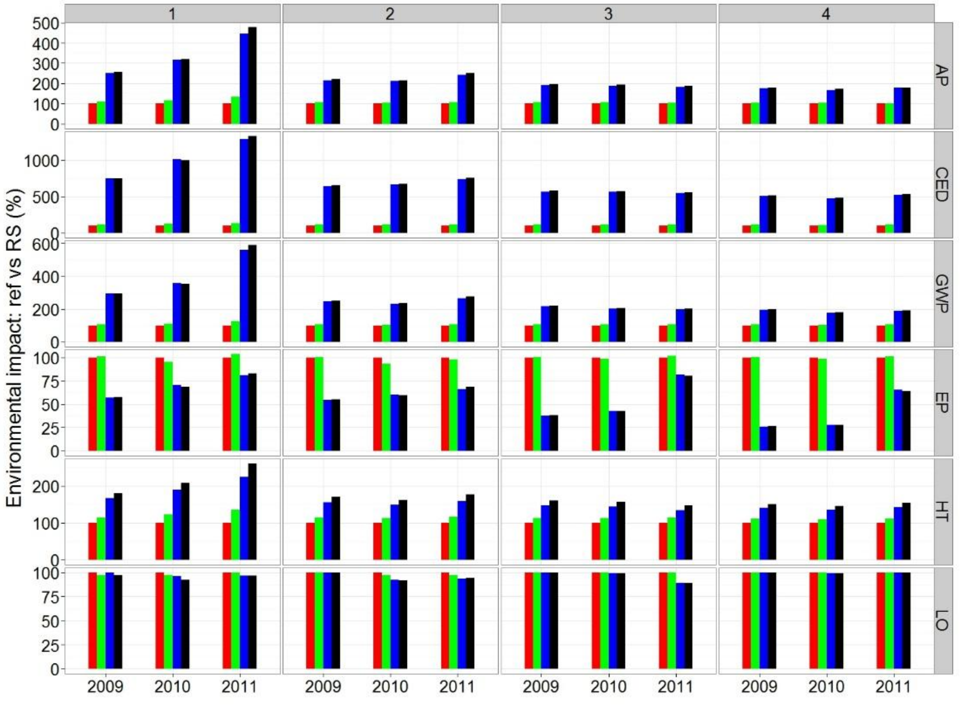

Figure 7-11 Relative environmental impact (acidification, AP; cumulative energy demand, CED; global warming, GWP; eutrophication, EP; human toxicity, HT and land occupation, LO) of the implemented reduction strategies (FF in green, SC in blue and FFSC in black)) compared to the reference system (in red) as estimated by the model based LCA regarding the rotation cycle in three consecutive years 2009-2011 under the four N dose treatments (1-4)

Next, in Figure 7-12, the relative impact share of the system components according to the strategy applied under the different N dose rates are shown, i.c. averaged over the years 2009-2011. These results are similar for each year, except for N dose 1 in 2011 which lack fertilizer production.

As the N dose rate increases, so do the impact share of fertilizer production and, if relevant, its use and inversely the auxiliary component for all systems considered. Whereas the auxiliary component accounts for 73.2%, 89.6%, 68.5%, 26.9% and 84.1% of respectively the AP, CED, GWP, EP and HT under N dose 1, it is reduced by half (a 3rd regarding CED) under N dose 4. Implementation of the strategy by FF, SC and FFSC however increases the auxiliary components share compared to the reference system by 26.4%, 133.1% and 142.7% regarding AP, by 12%, 90.5% and 90.9% regarding CED, by 23.3%, 202.8% and 207.9% regarding GWP, by 33.8%, 617% and 676.2% regarding EP and by 14.8%, 40.8% and 47.6% regarding HT.

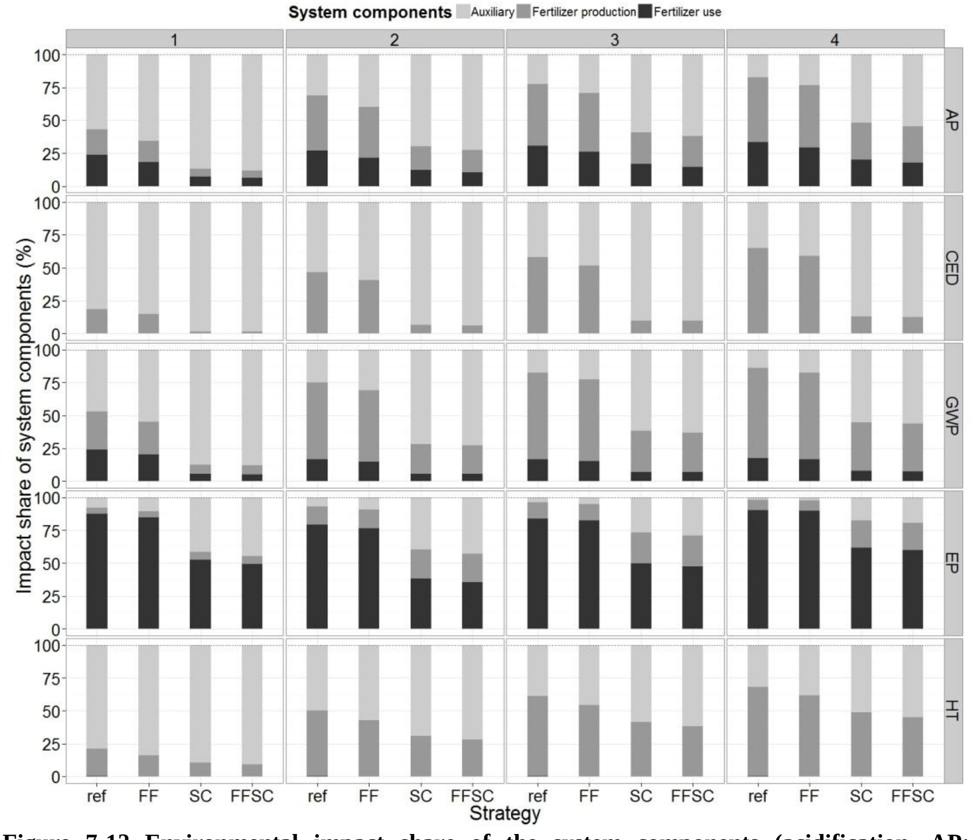

Figure 7-12 Environmental impact share of the system components (acidification, AP; cumulative energy demand, CED; global warming, GWP; eutrophication, EP; human toxicity, HT and land occupation, LO) as estimated by the model based LCA regarding the rotation cycle (averaged over the years 2009-2011) under the four N dose treatments (1-4) and according to reference system (ref) or the implemented reduction strategies (FF, SC and FFSC))

Life cycle interpretation

As shown, lowering the fertilizer input does not necessarily imply lower environmental impact. Low yields due to unfavourable conditions and/or inputs with high environmental burden can shift the outcome and preferred strategy, despite lower land occupation. As results are expressed as a function of the yield, results depend heavily on the change in inputs and the corresponding yield change. Within the boundaries defined, the assumptions made and the available databases regarding of the emissions along with the system processes applied for the current life cycle assessment, the environmental impact of the reduction strategy systems would be higher compared to that of the reference system. Main reason is the extra material and energy input to apply the reduction strategy which is not compensated (enough) by the expected yield increase and/or reduced field nitrogen emissions to benefit the environment. Besides the additional fertilizing operation with fractionated application, the impact of the auxiliary component, i.e.

plastic mulching with the SC and FFSC system is significant, as it is expected to be renewed every 2-3 years. As the amount is independent of the N dose rate applied, its contribution is higher with lower N dose.

The eutrophication potential however is an exception to the outcome as discussed as the impact of fertilizer use is generally still dominant. The absolute amounts of nitrogen prevented from leaching when applying a plastic mulch in winter fallow periods overcomes the eutrophication related to the auxiliary component, which is not valid regarding ammonia or nitrogen oxides causing acidification and global warming.

Ultimately, when considering the different reduction strategies it remains a trade-off between the impact categories. Although certain LCIA methods are available that normalize and even weigh the categories depending of the objective, the practitioner and/or the intended target, it is subjective and out of scope of this dissertation. If the assessment would be limited to nitrogen leaching and consequently the eutrophication, with the reduction as its primary and only goal, the LCA outcome shows that the reduction strategy, especially the implementation of the winter soil cover would indeed be beneficial, but meanwhile it would shift the problem towards acidification, energy use, global warming and human toxicity.

Chapter 8. Conclusion and perspectives

Horticulture faces mounting pressure to reduce its environmental impact, in particular nitrate leaching. Accurate evaluation is required to assess the burden and to support future management considering crop production and sustainability. Biological systems however are often complex, difficult to monitor and control. A key goal hereby is to pursue technical sustainability through understanding agriculture from a biophysical perspective in terms of water and nutrient dynamics and interactions among plant and soil under changing climate conditions. Maximum overall sustainability of a biological production system can only be realised if the technical sustainability and the related technical efficiency at field level are optimally controlled (Bojacá et al., 2012). A dynamic systems modelling framework is recommended as it is becoming a valuable tool for acquiring and increasing our scientific knowledge and enhancing sustainable crop production through innovative management strategies (Ahmed et al., 2013; Wallach et al., 2014). The development of agricultural modelling is still evolving in different disciplines, addressing different production systems from field, landscape, and beyond (Jones et al., 2017). Besides each model's contribution at its specific level and/or scale within a sustainability assessment, they can be combined in different ways to produce more comprehensive results that consider biophysical, socio-economic and environmental aspects.

8.1 The model based life cycle assessment approach

The present work provides an integrated dynamic and process based crop-soil model which is coupled to a life cycle assessment. This systems analysis approach contributes to the assessment of the technical sustainability of a biological production system. It responds to the call for the development of a generic methodological approach which can be adapted to the local context, includes descriptive information, simulation coding and evaluation performance criteria based on a test in practice (Bockstaller et al., 2009) , in particular the N fertilizer application management in a cauliflower-leek rotation cycle. The model simulates crop growth and development and soil water and nitrogen dynamics under varying climate conditions and different nitrogen fertilizer application rates. With this dynamic approach to predict the field nitrogen emissions, a more reliable and realistic assessment of the environmental impact can be obtained to enhance the by default static LCA output. Furthermore, the model based LCA allows the assessment of implications of future management scenarios considering potential impact reduction strategies.

Four main scientific queries were addressed considering the research questions formulated in section 0 towards the achievement stated above and discussed hereafter.

What is a commonly applied method to evaluate the environmental impact of a crop rotation system? What are the bottlenecks? What are the effects of different N dose rates over multiple years with varying climate?

→ ***Default life cycle assessment of the system with an empirical estimation approach regarding nitrogen field emissions***

The life cycle assessment quantified the environmental impact associated with the different fertilizer application rates for a cauliflower-leek rotation cycle for three consecutive years. The results as a function of the dry matter yield, showed an increased impact with increasing N dose rate, while land occupation decreased. When the *FRUIT* yield (i.e. curd of cauliflower and shaft of leek) was considered instead of the total yield, the differences were more pronounced but also occasionally in those three years led to better yield efficiency under lower N dose rates. The latter would be beneficial towards production and environmental impact compared to the commonly expected trade-off between total yield and environmental costs. Application of the LCA with an alternative functional unit, being the edible part of the crop yield, could be further assessed in a broader LCA study taken into account the nutritional value of the whole crop and the consumer phase. The ‘surplus’ yield of leaves that is sold along with the edible part of the crop usually ends up in a waste treatment, which often entails higher impacts (Nemecek et al., 2016).

Within the boundaries of the farm and agricultural operations accounted for, the fertilizer production and its application mostly dominated the auxiliary equipment and energy use. Due to the simplistic empirical approach of estimating nitrogen emissions closely related to fertilizer application, the LCA outcome furthermore suggest to reduce emissions through limiting inorganic fertilizer addition and/or avoiding crop residue incorporation from cauliflower as the nitrogen input is not compensated by the leek uptake that follows. Higher nitrogen losses are estimated in the summer fallow period between the two crop cultivations compared to the leaching in winter fallow periods, while the opposite or only the latter would be expected.

The aggregated level of field nitrogen emission estimations does not accord with the dynamic nature of highly variable nitrogen dynamics in a biological system. Furthermore, the empirical approach is limited to or cannot account for implications from different climate conditions or management strategies on crop growth or soil condition.

It is essential to find an appropriate assessment with system boundaries equally valid, both in agricultural practice and in the LCA model. Although LCA is praised for its holistic approach, it has an inherent static and linear nature and heavily depends on the quality of input data.

How does the crop growth integrate with soil water and nitrogen dynamics affected by varying weather and different fertilizer application rates?

→ ***Development of an integrated dynamic crop-soil model at field scale***

In order for the LCA to support decision-making towards more sustainable systems, an integrated crop-soil model was developed that simulates the nitrogen dynamics under varying climate conditions and different fertilizer applications.
The integrated model was developed to meet multiple demands:

- provide an improved insight in the system and allow more reliable predictions through simulation in combination with in situ measurements for calibration and validation
- understanding, quantifying and communicating the technical sustainability of products, processes and systems to continuously reducing their impacts and increasing their benefits to society
- address more complex questions including issues on sustainable production, environmental impacts and future strategies

Agro-ecosystem models are more and more applied to support decision-making at different scales, ranging from fertilizer recommendations for farms on a field scale up to a landscape or regional scale for strategic policy decision support (Jones et al., 2017). This work tries to respond to the challenges facing agricultural modelling in the 21st century as well articulated by the Agricultural Model Inter-comparison and Improvement Project (AgMip) protocols and pilot studies. They acknowledge the critical need for a model well suited operating with different conditions and relating soil water condition, carbon and nitrogen cycling, crop genetics and uptake, transient changes in climate and their interaction with management factors (Rosenzweig et al., 2013).
Model users and decision-makers also expect that the validity of models used has been proved, comparing non-calibrated modelling results with field observations outside the range of model development. A robust approach for crop simulation requires: (i) input data that meet minimum quality standards at the appropriate spatial scale, (ii) agronomic relevance with regard to cropping-system context, (iii) proper calibration and (iv) flexibility and transparency to account for different scenarios of data availability and quality (Grassini et al., 2015). This practical limit to the number of soil-crop climate conditions that can be addressed, led the present work to focus on open field vegetable production in Flanders, Belgium. However, while developing, future alternative options are accounted for through a modular approach, allowing for instance to implement other crops or improved equations that can handle different conditions more easily. Various overall models are mostly based on single submodels and also show overlap for some processes. Furthermore, more simplistic approaches due to limited access to data and aggregation of modules according to specific objectives are implemented. There is a need for modular systems with modules describing various processes with various levels of complexity. As calibration, let aside

validation, is often not addressed explicitly or limited to data visualisation, their performance could be questioned. In this work extensive calibration and validation was carried out on all process modules of the integrated model. Moreover, the R-code was developed in a modular way as all major processes were written as parameterized R-functions. This makes adaptations to other crops, soil and climate conditions very straightforward.

The presented model predicts on a daily basis the soil temperature, crop growth, water flow (interception, runoff, drain and deep percolation, evaporation, transpiration or uptake and diffusivity) and soil organic carbon and nitrogen dynamics (mineralisation or immobilisation, ammonium adsorption, ammonia volatilisation, (de)nitrification, leaching and uptake) including emissions of environmental pollutants to the air (i.e. ammonia, nitrous and nitric oxide) and to the ground water (i.e. nitrate). If the soil supply of water and/or nitrogen does not meet the demand of the crop, a deficiency factor is implemented to limit crop growth. The soil is divided in layers that can have different thicknesses and/or properties which have to be defined, next to the weather and the fertilizer and irrigation scheme. The model furthermore requires minimal information regarding geographical settings and initialisation of the soil content and crop cultivation.

With different degrees of development and application by the scientific and academic community, models involving alternative approaches to the one considered in this work, can be used within the context of sustainability in farming systems. The integration of the results of other or new methods applied to the biological production system under study with the ones obtained in this work may yield a more complete overview as no method can be considered as the only superior answer.

How is the model (performance) evaluated and optimized to address different conditions?

→ ***Calibration and validation of the model with experimental observations over multiple years under different N dose rates***

In order to implement the model to different contexts and assure adequate accuracy and reliability, it is necessary to test the sensitivity of the model over a wide range of diverse databases, and to elaborate correction functions taken into account the main explanatory factors of a process. It will serve as a more profound basis to conduct further improvements and implementation of the model on various case studies or future perspectives. Review of modelling research of agricultural processes show the lack of calibration and transparency and its poor applicability at another environment as data and model performance is not reported (Grassini et al., 2015).

Calibration

For this work, experiments were set up to monitor multiple cauliflower-leek rotations regarding crop growth and soil water and nitrogen contents under different N dose application rates. The model was calibrated for the first year of experiments and one reference N dose and validated with data of the subsequent two years and the other N dose rates respectively.

According to the visual match and the associated statistical indicators, model predictions for the calibration were very good. Given the large variability and strict performance rating thresholds, biomass growth, its nitrogen content, the water content and temperature in the different soil layers approached the observations very well. The soil nitrogen content however was considered satisfactory regarding nitrate, while ammonium content simulations suffered from the limited sampling numbers, the lack of detailed knowledge about adsorption for instance and the complex interaction of different pathways that affect the ammonium content simultaneously. More data points, especially for nitrogen content would have been desirable in order to improve fine-tuning. Unobserved flows of water and nitrogen like runoff or denitrification were purely simulated and fell overall within the literature ranges, merely to check the extent of scale as they exhibit large variability given the diversity on soil types, climate conditions, crop cultivation, in combination with different kinds of model implementations.

Along with the calibration, the sensitivity of model parameters was assessed to evaluate model responses. A fixed 10% change of the model parameters did not affect crop growth at both harvest times nor at the end of simulation. However certain soil processes were sensitive to a selection of parameters according to the ratio of their coefficients of variation. Especially runoff, water and nitrogen leaching and the emission of nitrous oxides showed a large variation in response to changes of mainly the runoff curve number for average moisture content and the water content at field capacity (of the top layer) among others.

Validation

The model (performance) was next evaluated under different conditions outside the calibration environment. Validation results for the other 2 years and the other 3 N dose rates respectively showed fair to (very) good results for crop growth regarding biomass and nitrogen accumulation with an occasional overestimation of the *FRUIT* in 2010 and of the fruit nitrogen content for the lowest N dose rate, although statistical indicators were often close to the performance rating thresholds. Also fair to good predictions of the soil water and temperature for the different soil layers were made in the subsequent years. However, the simulation of the soil nitrogen content, especially again regarding ammonium, showed poor validation results. To a certain extent the simulation of nitrogen contents does follow the trend that is seemingly set by the limited observations but it is not confirmed by the statistical indicators. Overall, a significant detrimental effect on yield potential due to a low nutrient application is confirmed. When no plant cover is present, severe leaching occurs reaching its maximum during the winter fallow period. Thus, careless pursuing higher yields through higher fertilizer application rates can quickly turn into environmental repercussions.

The complexity of multiple processes that interact influenced by the surrounding conditions of moisture and temperature in combination with their large variability and still lack of detailed knowledge explain the difficult task of model calibration and validation towards a wide applicable model. Appropriate calibration and validation allows better comparison of different model approaches for future applications and predictions under different conditions (Ahmed et al., 2013).

To what extent does the model enhance the environmental impact assessment and does the integrated approach contribute to the technical sustainability evaluation? What are the implications of future management?

→ ***Implementation of the dynamic model to support the default life cycle assessment and to run a scenario analysis involving potential impact reduction strategies***

One of the major shortcomings of LCA practice is the lack of consideration of the temporal and spatial variation of flows and emissions, and is still considered an unresolved problem and important limitation for the accuracy of LCA (McManus and Taylor, 2015). Broadly, in LCA, time can be taken into account at the level of the LCI, by modelling on a short- or long-term period and accounting for technology evolution and at the life cycle impact assessment (LCIA), by using characterisation functions based on time-dependent factors and/or by the optional normalisation and weighting of impacts, by for instance, discounting the impacts (Collet et al., 2014). In the current LCA framework, biological processes are assumed to respond linearly to environmental disturbances, and therefore, threshold effects are neglected. However, temporal factors (time of emissions and rate of release) have an effect on the impacts of pollution (Stasinopoulos et al., 2012). For instance, some impacts are subject to seasonal variations, such as aquatic eutrophication, which is higher in summer than in winter (Udo deHaes et al., 2002). Regardless the level of complexity considered, first of all the LCI must be dynamic, distributing the emissions and resource consumptions over time. The present work contributes to the dynamic LCA methodology, although for the time being, limited to the implicit study of the temporal changes in the processes as both emissions and impacts were still aggregated. Explicit methodologies, listed by Maier et al. (2017), include, among others, extrapolation of future developments, differentiating elementary and process flows over time with a structural path analysis, time-convolution and time-dependent characterisation factors. Along with weather forecasting, the model based LCA could fulfil a prospective analysis and future outlook for the agricultural system taking into account technological progress and/or evolutions in crop cultivars, etc.

Nevertheless, if the LCA needs to support future management decisions, an appropriate choice of approach for estimating field nitrogen emissions is required as it might shift the environmental favourable option to alternative and substantiated solutions, especially considering the timing of reduction strategy implementation. A daily time step and accounting for multiple processes and disturbing factors allows the model based simulation to provide more accurate and efficient adaptations towards sustainable systems, as addressed by the scenario analysis in this work. The implications of management adjustments or extreme climate changes on crop yield and nitrogen dynamics cannot be addressed by the default LCA method as the empirical approach depends on standard crop N uptake curves and does not account for precipitation and moisture effects for instance. The biophysical environment in which the agricultural process takes place, involves a series of interactions and relationships that limit the ability of the system to achieve its maximum performance. Once the management practices are optimised and carried out in an efficient way, considering the potential constraints of environmental soil and climate conditions, technical sustainability can be achieved (Bojacá et al., 2012).

Present case study

Overall, the model based LCA showed a consistently lower impact than the empirical based LCA results of the same crop rotation cycle and fertilizer management. The only exception was the eutrophication potential under the higher N dose application rates for all three years. Differences between the impacts according to both approaches tend to increase with increasing N dose rate besides the impact itself. Changes of impact over the different years were reflected similarly by both outcomes.

Looking at the field nitrogen emissions as such, the empirical estimation offers aggregated values for the whole period to a monthly distribution regarding nitrogen leaching, while the model based approach allows daily predictions. Each year a pattern in emissions is shown proportional to the N dose rate regarding the empirical approach, while this is less straightforward from the model based simulation. In contrast to the impact, differences between both estimations of field emissions regarding nitrate leaching and nitric oxide emissions are varying and respectively decreasing with increasing N dose rate. Whereas the model shows cumulatively lower ammonia volatilisation and nitrous oxide emissions compared to the empirical approach, the latter estimates lower nitric oxide emissions. Regarding nitrate leaching it depends on the N dose rate with higher leaching under higher N dose rates according to the model simulations compared to the empirical estimations.

Scenario analysis

Ultimately, future scenario analysis requires model simulations that can cope with the response of crop growth, soil processes and especially the nitrogen emissions to different management strategies, rather than the strategy as such. As a final chapter of this dissertation, the model based LCA was implemented for a scenario analysis that included potential reduction strategies regarding fractionated fertilizer application and plastic mulching during winter fallow periods. Whereas a fertilizer application distributed in time to meet the crop demand might reduce N stress and increase yield, the winter soil cover could prevent drain and subsequent nitrogen leaching. Although this was to a certain extent reflected in the outcome of the model simulations, the mitigated environmental impact regarding acidification, global warming, energy demand and human toxicity was turned around by the environmental burdens from additional fertilising equipment and energy use and/or especially from the plastic cover production and disposal. Only the eutrophication potential would be reduced if the strategy would be implemented. It shows that future decisions require a holistic perspective that combines dynamic model predictions and aggregated LCA results which still would imply a trade-off between different impacts, but would prevent the problem from merely shifting from one to the other.

The simulated impact effect from changes in environmental conditions and agricultural management should be considered as a potential effect that might be caused rather than the real impact reduction that can be expected in the future. The integrated model that has been developed still requires further improvement to match the observations in the first place under conditions different from the calibrated environment. Nevertheless, the model based approach does offer the ability to support future strategies aiming at more sustainable systems. Such scenario analysis is considered less reliable and could be more misleading with the empirical approach as applied in default LCA studies regarding dynamic agricultural systems. As yield is a common functional unit that affects heavily the outcome of an LCA, it should be predicted accurately. Furthermore, the simulation of soil water and nitrogen flows is crucial as the field nitrogen emissions are directly related and given the complex interactions of different processes influenced by the climate and soil conditions.

8.2 Future work

Along the presented research to address the objectives as discussed, new uncertainties and research gaps emerged.

An update to future technologies, materials and their associated characterisation factors that would imply less environmental impact might alter the outcome of the life cycle assessments. The experiments did involve besides the N dose rates also different fertilizer treatments like fertigation but were not yet incorporated in this thesis. From an LCA perspective fertigation would imply a shift from tractor use to a pump and tubing pipes of which polyethylene has a high environmental burden as shown regarding the plastic mulching. Characterisation of plastic recycling and recycled plastic as such or future bioplastic could be looked into. Observations did not confirm significant higher yields as expected with fertigation due to an optimized fertilizer application, temporal (to avoid N stress) and spatially (close to the plant roots). The nitrogen leaching under this treatment or any other treatment was highly uncertain. It would require better experimental monitoring and more detailed modelling efforts regarding root distribution and water transport to account for heterogeneity in a higher dimension. Research along these lines has however already been started by Vansteenkiste et al. (2014).

The presented model has been developed in a most generic way to allow adjustments towards alternative submodules. Once the basic parameters and initial values for other crops are known it should be fairly easy to incorporate them. Also for other submodules different approaches to simulate certain processes can be implemented to assess and compare their performance. Yet within the current submodules more simulation is still required to gain more insight, for instance on the temperature and moisture effect on soil nitrogen processes and the algorithm to deal with stress situations, especially regarding the response on crop growth and development.

Along with further simulation runs, the performance would benefit from sensitivity analysis on a multivariate level that allows the simultaneous change of different parameters. A long the same line, future work should include uncertainty analyses regarding the inherent variability of biological parameters instead of a fixed change and/or of auxiliary functions or driving variables like weather or initial state values. Furthermore, calibration and validation of the model could also be alternated with the different year and different N dose rates to optimize the model given the large variability of the system. Especially regarding the effect of N dose rate, further research should focus on water and nitrogen stress or excessive supply and how crop growth and the separate organ compartmentation is affected, e.g. root expansion or surplus storage respectively.

Next, more soil related assessments could complement the current work due to the heterogeneity of the soil and associated differences in texture, horizon segmentation and the sensitive characteristics regarding field capacity and bulk density. Furthermore, the potential sensitivity to soil layering should be looked into. It may require extended observations, yet simulations can already increase the knowledge and support further research.

To conclude, scenario options are limitless and current implementation of the model based life cycle assessment showed the strength and importance of a dynamic and process based system analysis to support future decisions towards more sustainability.

References

Abrahamsen, P. and Hansen, S. 2000. Daisy: an open soil-crop-atmosphere system model. Environ. Model. Softw. 15, 313–330. doi:10.1016/S1364-8152(00)00003-7

Acock, B., Charles-Edwards, D., Fitter, D.J., Hand, D., and Warren Wilson, J. 1978. Modelling canopy net photosynthesis by isolated blocks and rows of chrysanthemum plants. Ann. Appl. Biol. 90, 255–263.

Addiscott, T.M. and Whitmore, A.P. 1987. Computer simulation of changes in soil mineral nitrogen and crop nitrogen during autumn , winter and spring. J. Agric. Sci. 109, 141–157.

Aguilera, E., Lassaletta, L., Sanz-Cobena, A., Garnier, J., and Vallejo, A. 2013. The potential of organic fertilizers and water management to reduce N2O emissions in Mediterranean climate cropping systems. A review. Agric. Ecosyst. Environ. 164, 32–52. doi:10.1016/j.agee.2012.09.006

Ahmed, M., Asif, M., Hirani, A.H., Akram, M.N., and Goyal, A. 2013. Modeling for Agricultural Sustainability In: Agricultural Sustainability. Elsevier, pp. 127–147. doi:10.1016/B978-0-12-404560-6.00007-1

Allen, R.G., Pereira, L.S., Raes, D., and Smith, M. 1998. Crop Evapotranspiration - Guidelines for computing crop water requirements - FAO Irrigation and Drainage Paper No. 56.

Anonymous 1991. Council Directive of 12 december 1991 concerning the protection of waters against pollution caused by nitrates from agricultural sources (91/676/EEC). Off. J. Eur. Communities L375, 1–8.

AOAC 1999. Official methods of analysis, Method 968.06. Chapter 4. AOAC International, Gaithersburg, Md.

Asman, W.A.H. 1992. Ammonia emissions in Europe: updated emission and emission variations. Report 228471008. National institute of public health and environmental protection, Bilthoven, The Netherlands.

Aston, A.R. 1979. Rainfall interception by eight small trees. J. Hydrol. 42, 383–396.

Audsley, E., Alber, S., Cowell, S., Crettaz, P., Gaillard, G., Hausheer, J., Jolliet, O., Kleijn, R., Mortensen, B., Pearce, D., Roger, E., Teulon, H., Weidema, B.P., and van Zeijts, H. 1997. Harmonisation of environmental life cycle assessment. Final report, Concerted Action AIR3-CT94-2028. European Commision DG VI Agriculture.

Batelaan, O. and De Smedt, F. 2007. GIS-based recharge estimation by coupling surface–subsurface water balances. J. Hydrol. 337, 337–355. doi:10.1016/j.jhydrol.2007.02.001

Batlle-Aguilar, J., Brovelli, A., Porporato, A., and Barry, D.A. 2011. Modelling soil carbon and nitrogen cycles during land use change. A review. Agron. Sustain. Dev. 31, 251–274. doi:10.1051/agro/2010007

Baumann, D.T., Bastiaans, L., Goudriaan, J., Van Laar, H.H., and Kropff, M.J.

2002. Analysing crop yield and plant quality in an intercropping system using an eco-physiological model for interplant competition. Agric. Syst. 73, 173–203. doi:10.1016/S0308-521X(01)00084-1

Bausch, J.C., Bojórquez-Tapia, L., and Eakin, H. 2014. Agro-environmental sustainability assessment using multicriteria decision analysis and system analysis. Sustain. Sci. 9, 303–319. doi:10.1007/s11625-014-0243-y

Beaudoin, N., Saad, J.K., Van Laethem, C., Machet, J.M., Maucorps, J., and Mary, B. 2005. Nitrate leaching in intensive agriculture in Northern France: Effect of farming practices, soils and crop rotations. Agric. Ecosyst. Environ. 111, 292–310. doi:10.1016/j.agee.2005.06.006

Bennett, E.M., Carpenter, S.R., Gordon, L.J., Ramankutty, N., Balvanera, P., Campbell, B., Cramer, W., Foley, J., Folke, C., Karlberg, L., Liu, J., Lotze-Campen, H., Mueller, N.D., Peterson, G.D., Polasky, S., Rockström, J., Scholes, R.J., and Spierenburg, M. 2014. Toward a More Resilient Agriculture. Solut. a Sustain. desirable Futur. 5, 65–75.

Bessou, C., Lehuger, S., and Gabrielle, B. 2013a. Using a crop model to account for the effects of local factors on the LCA of sugar beet ethanol in Picardy region , France 24–36. doi:10.1007/s11367-012-0457-0

Bessou, C., Lehuger, S., Gabrielle, B., and Mary, B. 2012. Using a crop model to account for the effects of local factors on the LCA of sugar beet ethanol in Picardy region, France. Int. J. Life Cycle Assess. 18, 24–36. doi:10.1007/s11367-012-0457-0

Bessou, C., Lehuger, S., Gabrielle, B., and Mary, B. 2013b. Using a crop model to account for the effects of local factors on the LCA of sugar beet ethanol in Picardy region, France. Int. J. Life Cycle Assess. 18, 24–36. doi:10.1007/s11367-012-0457-0

Bessou, C., Mary, B., Léonard, J., Roussel, M., Gréhan, E., and Gabrielle, B. 2010. Modelling soil compaction impacts on nitrous oxide emissions in arable fields. Eur. J. Soil Sci. 61, 348–363. doi:10.1111/j.1365-2389.2010.01243.x

Björkman, O. 1981. Responses to Different Quantum Flux Densities In: Physiological Plant Ecology I. Springer Berlin Heidelberg, Berlin, Heidelberg, pp. 57–107. doi:10.1007/978-3-642-68090-8_4

Bockstaller, C. and Girardin, P. 2003. Mode de calcul des indicateurs agri-environnementaux de la méthode INDIGO (v.1.51 du logiciel).

Bockstaller, C., Guichard, L., Keichinger, O., Girardin, P., Galan, M., and Gaillard, G. 2009. Comparison of methods to assess the sustainability of agricultural systems. A review. Agron. Sustain. Dev. 29, 223–235. doi:10.1051/agro:2008058

Bojacá, C.R. 2009. Generic modelling approaches to technical sustainability assessment on field level for farming systems in the high andean tropics. PhD dissertation, Faculty of Bioscience Engineering. KU Leuven, Belgium.

Bojacá, C.R., García, S.J., and Schrevens, E. 2012. Investigating the technical sustainability of farming systems with correlational biplots. Int. J. Sustain.

Dev. World Ecol. 19, 361–368. doi:10.1080/13504509.2012.671194
Bojacá, C.R., Wyckhuys, K.A.G., and Schrevens, E. 2014. Life cycle assessment of Colombian greenhouse tomato production based on farmer-level survey data. J. Clean. Prod. 69, 26–33. doi:10.1016/j.jclepro.2014.01.078
Boldrin, A., Andersen, J.K., Møller, J., Christensen, T.H., and Favoino, E. 2009. Composting and compost utilization: Accounting of greenhouse gases and global warming contributions. Waste Manag. Res. 27, 800–812. doi:10.1177/0734242X09345275
Bosco, S., Bene, C., Galli, M., Remorini, D., Massai, R., and Bonari, E. 2013. Soil organic matter accounting in the carbon footprint analysis of the wine chain. Int. J. Life Cycle Assess. 18, 973–989. doi:10.1007/s11367-013-0567-3
Bouraoui, F., Billen, G., Grinsven, H. Van, Cardoso, A.C., Th, V., Garnier, J., Curtis, C., Howarth, R., and Johnes, P. 2011. Nitrogen as a threat to European water quality In: Sutton, M.A. (ed.), The European Nitrogen Assessment. Cambridge University Press, pp. 379–404.
Bouwman, A.F., Boumans, L.J.M., and Batjes, N.H. 2002a. Emissions of N 2 O and NO from fertilized fields: Summary of available measurement data. Global Biogeochem. Cycles 16, 6-1-6–13. doi:10.1029/2001GB001811
Bouwman, A.F., Boumans, L.J.M., and Batjes, N.H. 2002b. Modeling global annual N 2 O and NO emissions from fertilized fields. Global Biogeochem. Cycles 16, 28-1-28–9. doi:10.1029/2001GB001812
Bradbury, N.J., Whitmore, A.P., Hart, P.B.S., and Jenkinson, D.S. 1993a. Modelling the fate of nitrogen in crop and soil in the years following application of 15N-labelled fertilizer to winter wheat. J. Agric. Sci. 121, 363. doi:10.1017/S0021859600085567
Bradbury, N.J., Whitmore, a. P., Hart, P.B.S., and Jenkinson, D.S. 1993b. Modelling the fate of nitrogen in crop and soil in the years following application of 15N-labelled fertilizer to winter wheat. J. Agric. Sci. 121, 363. doi:10.1017/S0021859600085567
Brentrup, F., Kiisters, J., Lammel, J., and Kuhlmann, H. 2000. Methods to estimate on-field nitrogen emissions from crop production as an input to LCA studies in the agricultural sector. Int. J. LCA 5, 349–357.
Brisson, N., Gary, C., Justes, E., Roche, R., Mary, B., Ripoche, D., Zimmer, D., Sierra, J., Bertuzzi, P., Burger, P., Bussiere, F., Cabidoche, Y.M., Cellier, P., Debaeke, P., Gaudillere, J.P., Hénault, C., Maraux, F., Seguin, B., and Sinoquet, H. 2003. An overview of the crop model STICS. Eur. J. Agron. 18, 309–332.
Brouwers, J., De Geest, C., Devriendt, S., Peeters, B., Struyf, I., Vancraeynest, L., Vander Putten, E., Vandevenne, F., Van Hooste, H., and Van Steertegem, M. 2017. Systeembalans 2017: Milieuuitdagingen voor het energie-, mobiliteits- en voedingssyteem in Vlaanderen. Milieurapport Vlaanderen - MIRA. Aalst, Vlaamse milieumaatschappij (VMM).
Brouwers, J., Peeters, B., Van Steertegem, M., van Lipzig, N., Wouters, H.,

Beullens, J., Demuzere, M., Willems, P., De Ridder, K., Maiheu, B., De Troch, R., Termonia, P., Vansteenkiste, T., Craninx, M., Maetens, W., Defloor, W., and Cauwenberghs, K. 2015. MIRA Klimaatrapport 2015, over waargenomen en toekomstige klimaatveranderingen. Vlaamse Milieumaatschappij i.s.m. KU Leuven, VITO en KMI. Aalst, Belgium, 147p.

BURNS, I.G. 1974. A model for predicting the redistribution of salts applied to fallow soils after excess rainfall or evaporation. J. Soil Sci. 25, 165–178. doi:10.1111/j.1365-2389.1974.tb01113.x

Butchee, K.S., May, J., and Arnall, B. 2011. Sensor based nitrogen management reduced nitrogen and maintained yield. Crop Manag. CM-2011-0725-01-RS. doi:10.1094/CM-2011-0725-01-RS.Abstract

Cannavo, P., Recous, S., Parnaudeau, V., and Reau, R. 2008. Modeling N dynamics to assess environmental impacts of cropped soils In: Advances in Agronomy. pp. 131–174.

Cederberg, C. 2010. Improving nutrient management in agriculture to reduce eutrophication, acidification and climate change In: Environmental Assessment and Management in the Food Industry. Elsevier, pp. 3–15. doi:10.1533/9780857090225.1.3

Coleman, K. and Jenkinson, D.S. 1999. RothC-26.3 A model for the turnover of carbon in soil. Model description and windows users guide. November 1999 issue. IACR - Rothamsted.

Collet, P., Lardon, L., Steyer, J.-P., and Hélias, A. 2014. How to take time into account in the inventory step: a selective introduction based on sensitivity analysis. Int. J. Life Cycle Assess. 19, 320–330. doi:10.1007/s11367-013-0636-7

Constantin, J., Beaudoin, N., Launay, M., Duval, J., and Mary, B. 2012. Long-term nitrogen dynamics in various catch crop scenarios: Test and simulations with STICS model in a temperate climate. Agric. Ecosyst. Environ. 147, 36–46. doi:10.1016/j.agee.2011.06.006

Cooman, A. 2002. Feasibility of protected tomato cropping in the high altitude tropics using statistical and system dynamic models for plant growth and development. PhD Thesis, KU Leuven.

Dane, J.H. and Hopmans, J.W. 2002. Soil water retention and storage. In: Dane, J.H., Topp, G.C. (eds.), Methods of Soil Analysis. Part 4 Physical Methods. Soil science society of America, Wisconsin, USA., pp. 671–674.

Dayan, E., van Keulen, H., Jones, J.W., Zipori, I., Shmuel, D., and Challa, H. 1993. Development, calibration and validation of a greenhouse tomato growth model: I. Description of the model. Agric. Syst. 43, 145–163. doi:10.1016/0308-521X(93)90024-V

de Jong, S.M. and Jetten, V.G. 2007a. Estimating spatial patterns of rainfall interception from remotely sensed vegetation indices and spectral mixture analysis. Int. J. Geogr. Inf. Sci. 21, 529–545. doi:10.1080/13658810601064884 de Jong, S.M. and Jetten, V.G. 2007b. Estimating spatial patterns of rainfall interception from remotely sensed vegetation indices and spectral mixture analysis. Int. J. Geogr. Inf. Sci. 21, 529–545. doi:10.1080/13658810601064884

DeJong, T.M. 1982. Leaf nitrogen content and CO2 assimilation capacity in peach. J. Am. Soc. Hortic. Sci., Journal of the American Society for Horticultural Science 107, 955–959.

DeJonge, K.C., Ascough, J.C., Andales, A.A., Hansen, N.C., Garcia, L.A., and Arabi, M. 2012. Improving evapotranspiration simulations in the CERES-Maize model under limited irrigation. Agric. Water Manag. 115, 92–103. doi:10.1016/j.agwat.2012.08.013

EEA 2010. The European environment: state and outlook 2010: Freshwater quality In: Collins, R. (ed.), SOER 2010: Thematic Assessments. European Environment Agency (EEA), Copenhagen, Denmark. doi:10.2800/60214

EMIS 2010. Bodem - Bepaling van nitraatstikstof. BAM - Bemonsterings- en analysemethodes voor bodem in het kader van het mestdecreet.

Erisman, J.W., van Grinsven, H., Grizetti, B., Bouraoui, F., Powlson, D., Sutton, M.A., Bleeker, A., and Reis, S. 2011. The European nitrogen problem in a global perspective. In: Sutton, M.A., Howard, C.M., Erisman, J.W., Billen, G., Bleeker, A., Grennfelt, P., Van Grinsven, H., Grizzetti, B. (eds.), The European Nitrogen Assessment (ENA). Cambridge University Press, Cambridge, p. 664.

European Commission 2015. EU ETS Handbook, Climate Action. doi:10.2834/55480

Evett, S.R. 2003. Soil Water Measurement by Time Domain Reflectometry. Water 894–898. doi:10.1081/E-EWS

Falloon, P., Smith, P., Coleman, K., and Marshall, S. 1998. Estimating the size of the inert organic matter pool from total soil organic carbon content for use in the Rothamsted carbon model. Soil Biol. Biochem. 30, 1207–1211.

FAO 2013. SAFA Sustainability assessment of food and agriculture systems. Guidelines v 3.0. doi:10.2144/000113056

Feller, C., Fink, M., Laber, H., Mayne, A., Paschold, P.-J., Scharpf, H.-C., Schlaghecken, J., Strohmeyer, K., Weier, U., and Ziegler, J. 2011. Düngung im Freilandgemüsebau. In: Schriftenreihe Des Leibniz-Institus Für Gemüse- Und Zierpflanzenbau (IGZ), 3. Auflage, Heft 4. Grosbeeren.

Finnveden, G., Hauschild, M.Z., Ekvall, T., Guinée, J., Heijungs, R., Hellweg, S., Koehler, A., Pennington, D., and Suh, S. 2009. Recent developments in Life Cycle Assessment. J. Environ. Manage. 91, 1–21. doi:10.1016/j.jenvman.2009.06.018

Foley, J.A., Ramankutty, N., Brauman, K.A., Cassidy, E.S., Gerber, J.S., Johnston, M., Mueller, N.D., O'Connell, C., Ray, D.K., West, P.C., Balzer, C., Bennett, E.M., Carpenter, S.R., Hill, J., Monfreda, C., Polasky, S., Rockström, J., Sheehan, J., Siebert, S., Tilman, D., and Zaks, D.P.M. 2011. Solutions for a cultivated planet. Nature 478, 337–342.

doi:10.1038/nature10452
Frischknecht, R., Jungbluth, N., Althaus, H.-J., Doka, G., Dones, R., Heck, T., Hellweg, S., Hischier, R., Nemecek, T., Rebitzer, G., and Spielmann, M. 2005. The ecoinvent Database: Overview and Methodological Framework (7 pp). Int. J. Life Cycle Assess. 10, 3–9. doi:10.1065/lca2004.10.181.1
Génermont, S. and Cellier, P. 1997. A mechanistic model for estimating ammonia volatilization from slurry applied to bare soil. Agric. For. Meteorol. 88, 145–167. doi:10.1016/S0168-1923(97)00044-0
Geypens, M. and Vandendriessche, H. 1996. Advisory systems for nitrogen fertilizer recommendations. Plant Soil 181, 31–38. doi:10.1007/BF00011289
Giltrap, D.L., Li, C., and Saggar, S. 2010. DNDC: A process-based model of greenhouse gas fluxes from agricultural soils. Agric. Ecosyst. Environ. 136, 292–300. doi:10.1016/j.agee.2009.06.014
Godfray, H.C.J., Beddington, J.R., Crute, I.R., Haddad, L., Lawrence, D., Muir, J.F., Pretty, J., Robinson, S., Thomas, S.M., and Toulmin, C. 2010. Food Security: The Challenge of Feeding 9 Billion People. Science (80-.). 327, 812–818. doi:10.1126/science.1185383
Grassini, P., van Bussel, L.G.J., Van Wart, J., Wolf, J., Claessens, L., Yang, H., Boogaard, H., de Groot, H., van Ittersum, M.K., and Cassman, K.G. 2015. How good is good enough? Data requirements for reliable crop yield simulations and yield-gap analysis. F. Crop. Res. 177, 49–63. doi:10.1016/j.fcr.2015.03.004
Gruber, V., Holweg, C., and Teller, C. 2016. What a Waste! Exploring the Human Reality of Food Waste from the Store Manager's Perspective. J. Public Policy Mark. 35, 3–25. doi:10.1509/jppm.14.095
Guinée, J.B., Gorrée, M., Heijungs, R., Huppes, G., Kleijn, R., de Koning, a., van Oers, L., Wegener Sleeswijk, A., Suh, S., Udo de Haes, H.A., de Bruijn, H., van Duin, R., and Huijbregts, M.A.J. 2002. Handbook on life cycle assessment. Operational guide to the ISO standards. I: LCA in perspective. IIa: Guide. IIb: Operational annex. III: Scientific background. Kluwer Academic Publishers, Dordrecht.
Guo, M., Li, C., Bell, J.N.B., and Murphy, R.J. 2012. Influence of agro-ecosystem modeling approach on the greenhouse gas profiles of wheat-derived biopolymer products. Environ. Sci. Technol. 46, 320–30. doi:10.1021/es2030388
Harris, S. and Narayanaswamy, V. 2009. A Literature Review of Life Cycle Assessment in Agriculture. Australian Government, Rural Industries Research and Development Corporation (RIRDC).
Harrison, R. and Webb, J. 2001. A review of the effect of N fertilizer type on gaseous emissions In: Advances in Agronomy. pp. 65–108. doi:10.1016/S0065-2113(01)73005-2
Hayashi, K., Gaillard, G., and Nemecek, T. 2006. LIFE CYCLE ASSESSMENT OF AGRICULTURAL PRODUCTION SYSTEMS : In: Good Agricultural Practice (GAP) in Asia and Oceania. Food and Fertilizer Technology

Center, Taipei, pp. 98–110.
Hayati, D., Ranjbar, Z., and Karami, E. 2010. Measuring Agricultural Sustainability. Biodiversity, Biofuels, Agrofor. Conserv. Agric. Sustain. Agric. Rev. 5. doi:10.1007/978-90-481-9513-8
Heirman, J.-P. 2011. Milieubeleidsplan 2011-2015.
Henault, C., Bizouard, F., Laville, P., Gabrielle, B., Nicoullaud, B., Germon, J.C., and Cellier, P. 2005. Predicting in situ soil N2O emission using NOE algorithm and soil database. Glob. Chang. Biol. 11, 115–127. doi:10.1111/j.1365-2486.2004.00879.x
Hirose, T., Lambers, H., Konings, H., and Werf, A. Van Der 1989. Modelling of Respiration: Effect of Variation in Respiration on Plant Growth in Two Carex Species. Funct. Ecol. 3, 655. doi:10.2307/2389497
Hoogenboom, G., Jones, J.., Wilkens, P.., Porter, C.., Boote, K.., Hunt, L.., Singh, U., Lizaso, J.., White, J.., Uryasev, O., Ogoshi, R., Koo, J., Shelia, V., and Tsuji, G.. 2015. Decision Support System for Agrotechnology Transfer (DSSAT) Version 4.6 (www.DSSAT.net). DSSAT Foundation, Prosser, Washington.
IPCC 2006. 2006 IPCC Guidelines for National greenhouse gas inventories. Prepared by the National greenhouse gas inventories programme. Eggleston H.S., Buendia L., Miwa K., Ngara T. and Tanabe K. (eds). Published by IGES, Japan.
ISO 2006. ISO 14040:2006 Environmental management. Life cycle asssessment. Principles and framework.
Jenkinson, D.S. and Coleman, K. 2008. The turnover of organic carbon in subsoils. Part 2. Modelling carbon turnover. Eur. J. Soil Sci. 59, 400–413. doi:10.1111/j.1365-2389.2008.01026.x
Jenkinson, D.S., Hart, P.B.S., Rayner, J.H., and Parry, L.C. 1987. Modelling the turnover of organic matter in long-term experiments at Rothamsted In: Cooley, J.H. (ed.), Soil Organic Matter Dynamics and Soil Productivity. Athens. International Association for Ecology, pp. 1–8.
Jeuffroy, M.H., Ney, B., and Ourry, A. 2002. Integrated physiological and agronomic modelling of N capture and use within the plant. J. Exp. Bot. 53, 809–23.
Jia-Fang, C. 1997. Adsorption and diffusion of ammonium in soils. In: Zhao-liang, Z., Qi-xiao, W. and Freney, J.. (ed.), Nitrogen in Soils of China. Kluwer Academic Publishers.
Johnson, B. and Villumsen, G. 2018. Environmental aspects of natural resource intensive development: the case of agriculture. Innov. Dev. 8, 167–188. doi:10.1080/2157930X.2017.1317915
Jones, C.A. and Kiniry, J.R. 1986. CERES-Maize. A simulation model of maize growth and development. Texas A&M University Press.
Jones, J.W., Antle, J.M., Basso, B., Boote, K.J., Conant, R.T., Foster, I., Godfray, H.C.J., Herrero, M., Howitt, R.E., Janssen, S., Keating, B.A., Munoz-Carpena, R., Porter, C.H., Rosenzweig, C., and Wheeler, T.R. 2017. Brief

history of agricultural systems modeling. Agric. Syst. 155, 240–254. doi:10.1016/j.agsy.2016.05.014
Jones, J.W., Dayan, E., Van Keulen, H., and Challa, H. 1989. Modeling tomato growth for optimizing greenhouse temperatures and carbon dioxide concentrations. Acta Hort 248.
Jones, J.W., Hoogenboom, G., Porter, C.H., Boote, K.J., Batchelor, W.D., Hunt, L.A., Wilkens, P.W., Singh, U., Gijsman, A.J., and Ritchie, J.T. 2003. The DSSAT cropping system model.
Jorgensen, M.S., Detlefsen, N.K., and Hutchings, N.J. 2005. FarmN: A decision support tool for managing Nitrogen flow at the farm level In: 5th Conference of the European Federation for Information Technology in Agriculture, Food and Environment. Vila Real, Portugal, pp. 67–73.
Jury, W.A. and Horton, R. 2004. Soil physics, 6th edition. John Wiley and Sons Ltd, New York.
Keating, B.A., Carberry, P.S., Hammer, G.L., Probert, M.E., Robertson, M.J., Holzworth, D., Huth, N.I., and Hargrea, J.N.G. 2003. An o v er v iew of APSIM , a model designed for farming systems simulation 18.
Kemanian, A.R., Stöckle, C.O., and Huggins, D.R. 2005. Transpiration-use efficiency of barley. Agric. For. Meteorol. 130, 1–11. doi:10.1016/j.agrformet.2005.01.003
Kersebaum, K.C., Hecker, J.-M., Mirschel, W., and Wegehenkel, M. 2004. Modelling water and nutrient dynamics in soil-crop systems. Proceedings of the Workshop on “Modelling water and nutrient dynamics in soil-crop systems” held on 14-16 June 2004. Muncheberg, Germany.
Kimura, K., Kikuchi, S., and Yamasaki, S. 1999. No Title. Plant Soil 216, 117–127. doi:10.1023/A:1004778925316
Kozak, J.A., Ahuja, L.R., Green, T.R., and Ma, L. 2007. Modelling crop canopy and residue rainfall interception effects on soil hydrological components for semi-arid agriculture. Hydrol. Process. 21, 229–241. doi:10.1002/hyp.6235
Le Gal, P.-Y., Merot, a., Moulin, C.-H., Navarrete, M., and Wery, J. 2010. A modelling framework to support farmers in designing agricultural production systems. Environ. Model. Softw. 25, 258–268. doi:10.1016/j.envsoft.2008.12.013
Legates, D. and Mccabe, G.-J.J. 1999. Evaluating the use of “goodness-of-fit” measures in hydrologic and hydroclimatic model validation. Water Resour. Res. 35, 233–241.
Lenders, S. and Deuninck, J. 2016. Gebruik van energie, gewasbescherming, water en kunstmest in de vlaamse landbouw 35.
Li, C., Farahbakhshazad, N., Jaynes, D.B., Dinnes, D.L., Salas, W., and McLaughlin, D. 2006. Modeling nitrate leaching with a biogeochemical model modified based on observations in a row-crop field in Iowa. Ecol. Modell. 196, 116–130. doi:10.1016/j.ecolmodel.2006.02.007
Liu, S., Yang, J.Y., Zhang, X.Y., Drury, C.F., Reynolds, W.D., and Hoogenboom, G. 2013. Modelling crop yield , soil water content and soil temperature for a

soybean – maize rotation under conventional and conservation tillage systems in Northeast China. Agric. Water Manag. 123, 32–44. doi:10.1016/j.agwat.2013.03.001

Lorenz, H., Schlagenhecken, J., and Engl, G. 1985. Gezielte Stickstoffversorgung. Das Kulturbegeleitende Nmin-Sollwerte System. Dtsch. Gartenbau 13, 646–648.

Maier, M., Mueller, M., and Yan, X. 2017. Introducing a localised spatio-temporal LCI method with wheat production as exploratory case study. J. Clean. Prod. 140, 492–501. doi:10.1016/j.jclepro.2016.07.160

Martínez-Blanco, J., Muñoz, P., Antón, A., and Rieradevall, J. 2011. Assessment of tomato Mediterranean production in open-field and standard multi-tunnel greenhouse, with compost or mineral fertilizers, from an agricultural and environmental standpoint. J. Clean. Prod. 19, 985–997. doi:10.1016/j.jclepro.2010.11.018

McManus, M.C. and Taylor, C.M. 2015. The changing nature of life cycle assessment. Biomass and Bioenergy 82, 13–26. doi:10.1016/j.biombioe.2015.04.024

Merriam, R.A. 1960. A note on the interception loss equation. J. Geophys. Res. 65, 3850–3851. doi:10.1029/JZ065i011p03850

Milà i Canals, L., Muñoz, I., Hospido, A., Plassmann, K., and Mclaren, S. 2008a. LIFE CYCLE ASSESSMENT (LCA) OF DOMESTIC VS . IMPORTED VEGETABLES . Case studies on broccoli , salad crops and green beans. Rural Economy and Land use (RELU) programme funded project.

Milà i Canals, L., Muñoz, I., Hospido, A., Plassmann, K., and McLaren, S. 2008b. Life Cycle Assessment (LCA) of domestic vs. imported vegetables. Case studies on broccoli, salad crops and green beans. United Kingdom, Cent. Environ. Strateg. Univ. Surrey 46. doi:1464-8083

Misselbrook, T.H., Misselbrook, T.H., Sutton, M.A., and Scholefield, D. 2004. A simple process-based model for estimating ammonia emissions from agricultural land after fertilizer applications. Soil Use Manag. 20, 365–372. doi:10.1079/SUM2004280

Monod, H., Naud, C., and Makowski, D. 2006. Uncertainty and sensitivity analysis for crop models. In: Wallach, D., Makowski, D., Jones, J.W. (eds.), Working with Dynamic Crop Models. Elsevier B.V., Amsterdam, The Netherlands, pp. 55–100.

Mooney, H.A. and Gulmon, S.L. 1979. Environmental and Evolutionary Constraints on the Photosynthetic Characteristics of Higher Plants In: Topics in Plant Population Biology. Macmillan Education UK, London, pp. 316–337. doi:10.1007/978-1-349-04627-0_14

Moriasi, D.N., Arnold, J.G., Van Liew, M.W., Bingner, R.L., Harmel, R.D., and Veith, T.L. 2007. Model Evaluation Guidelines for Systematic Quantification of Accuracy in Watershed Simulations. Trans. ASABE 50, 885–900. doi:10.13031/2013.23153

Nash, J. and Sutcliffe, J. 1970. River flow forecasting through conceptual models.

Part I. A discussion of principles. J. Hydrol. 10, 282–290.
Neitsch, S., Arnold, J., Kiniry, J., and Williams, J. 2011. Soil & Water Assessment Tool Theoretical Documentation Version 2009. Texas Water Resources Institute Technical Report No. 406, Texas.
Nemecek, T. and Erzinger, S. 2005. Modelling Representative Life Cycle Inventories for Swiss Arable Crops (9 pp). Int. J. Life Cycle Assess. 10, 68–76. doi:10.1065/lca2004.09.181.8
Nemecek, T., Frick, C., Dubois, D., and Gaillard, G. 2001. Comparing farming systems at crop rotation level by LCA In: Geerken, T., Mattson, B., Olsson, P., Johansson, E. (eds.), Proceedings of the International Conference on LCA in Foods. Gothenburg, Sweden, pp. 65–69.
Nemecek, T., Jungbluth, N., i Canals, L.M., and Schenck, R. 2016. Environmental impacts of food consumption and nutrition: where are we and what is next? Int. J. Life Cycle Assess. 21, 607–620. doi:10.1007/s11367-016-1071-3
Nemecek, T. and Kägi, T. 2007. Life Cycle Inventories of Agricultural Production Systems. Ecoinvent report No. 15. Ecoinvent Centre - Swiss centre for life cycle inventories. Zürich and Dübendorf, December 2007.
Nemecek, T. and Schnetzer, J. 2011. Methods of assessment of direct field emissions for LCIs of agricultural production systems. Data v. 3.0, Ecoinvent Reports. Zurich.
Nemecek, T. and Schnetzer, J. 2012. Methods of assessment of direct field emissions for LCIs of agricultural production systems. Data v3.0. Zurich.
Ness, B., Urbel-Piirsalu, E., Anderberg, S., and Olsson, L. 2007. Categorising tools for sustainability assessment. Ecol. Econ. 60, 498–508. doi:10.1016/j.ecolecon.2006.07.023
Notarnicola, B., Sala, S., Anton, A., McLaren, S.J., Saouter, E., and Sonesson, U. 2017. The role of life cycle assessment in supporting sustainable agri-food systems: A review of the challenges. J. Clean. Prod. 140, 399–409. doi:10.1016/j.jclepro.2016.06.071
Olesen, J.E. and Grevsen, K. 1997. Effects of temperature and irradiance on vegetative growth of cauliflower (Brassica oleracea L. botrytis) and broccoli (Brassica oleracea L. italica). J. Exp. Bot. 48, 1591–1598. doi:10.1093/jxb/48.8.1591
Park, C. 2012. VELAS: a fully distributed daily hydrologic feedback model with emphasis on vegetation, land cover and soil water dynamics. A dissertation in Geosciences and Computer Science. Kansas City, Missouri.
Parton, W.J., Scurlock, J.M.O., Ojima, D.S., Gilmanov, T.G., Scholes, R.J., Qchimel, D.S., Kirchner, T., Menaut, J.-C., Seastedt, T., Garcia, E., Kamnalrut, A., and Kinyamario, J.I. 1993. Observations and modeling of biomass and soil organic matter dynamics for the grassland biome worldwide. Global Biogeochem. Cycles 7, 785–809.
Payraudeau, S. 2007. Analysis of the uncertainty associated with the estimation of nitrogen losses from farming systems 94, 416–430.

doi:10.1016/j.agsy.2006.11.014

Pedersen, A., Zhang, K., Thorup-Kristensen, K., and Jensen, L.S. 2010. Modelling diverse root density dynamics and deep nitrogen uptake—A simple approach. Plant Soil 326, 493–510. doi:10.1007/s11104-009-0028-8

Penning de Vries, F.W.T. 1975. The Cost of Maintenance Processes in Plant Cells. Ann. Bot. 39, 77–92. doi:10.1093/oxfordjournals.aob.a084919

Perrin, A., Basset-Mens, C., and Gabrielle, B. 2014. Life cycle assessment of vegetable products: a review focusing on cropping systems diversity and the estimation of field emissions. Int. J. Life Cycle Assess. 19, 1247–1263. doi:10.1007/s11367-014-0724-3

Peter, C., Fiore, A., Hagemann, U., Nendel, C., and Xiloyannis, C. 2016. Improving the accounting of field emissions in the carbon footprint of agricultural products: a comparison of default IPCC methods with readily available medium-effort modeling approaches. Int. J. Life Cycle Assess. 21, 791–805. doi:10.1007/s11367-016-1056-2

Platteau, J., Van Gijseghem, D., and Van Bogaert, T. 2014. LARA 2014 Landbouwrapport. Departement Landbouw en Visserij., Brussel.

Platteau, J., Van Gijseghem, D., Van Bogaert, T., and Vuylsteke, A. 2016. Voedsel om over na te denken. Landbouw- en visserijrapport 2016. Departement Landbouw en Visserij. Brussel.

R Core Team 2016. R: a language and environment for statistical computing. R foundation for Statistical Computing.

R Development Core Team 2015. R: A language and environment for statistical computing. R Foundation for Statistical Computing, Vienna, Austria.

Raes, D., Steduto, P., Hsiao, T.C., and Fereres, E. 2009. AquaCrop — The FAO Crop Model to Simulate Yield Response to Water: II. Main Algorithms and Software Description. doi:10.2134/agronj2008.0140s

Rahn, C.R., Zhang, K., Lillywhite, R., Ramos, C., Doltra, J., Paz, J.M. De, Riley, H., Fink, M., Nendel, C., Kristensen, K.T., Pedersen, A., Piro, F., Venezia, A., Firth, C., Schmutz, U., Rayns, F., Hri, W., Inves-, I.V. De, Ivia, A., Superior, C., and Científicas, D.I. 2010. EU-Rotate _ N – a European Decision Support System – to Predict Environmental and Economic Consequences of the Management of Nitrogen Fertiliser in Crop Rotations. Eur. J. Hortic. Sci. 75, 20–32.

Regina, K., Kaseva, J., and Esala, M. 2013. Emissions of nitrous oxide from boreal agricultural mineral soils—Statistical models based on measurements. Agric. Ecosyst. Environ. 164, 131–136. doi:10.1016/j.agee.2012.09.013

Richner, W., Oberholzer, H., Freiermuth, R., Huguenin, O., Ott, S., Nemecek, T., and Walther, U. 2014. Modell zur Beurteilung der Nitratauswaschung in Ökobilanzen – SALCA-NO3. Unter Berücksichtigung der Bewirtschaftung (Fruchtfolge, Bodenbearbeitung, N-Düngung), der mikrobiellen Nitratbildung im Boden, der Stickstoffaufnahme durch die Pflanzen und verschie. Agroscope Sci. 5, 60.

Ritchie, J.T. 1998. Soil water balance and plant water stress In: Tsuji, G.., Hoogenboom, G., Thorton, P.K. (eds.), Understanding Options for Agricultural Production. Systems Appraoches for Sustainable Agricultural Development. Springer, Dordrecht, pp. 41–54. doi:10.1007/978-94-017-3624-4_3

Ritchie, J.T., Porter, C.H., Jones, J.W., and Suleiman, A.A. 2009. Extension of an Existing Model for Soil Water Evaporation and Redistribution under High Water Content Conditions 73. doi:10.2136/sssaj2007.0325

Rockström, J., Williams, J., Daily, G., Noble, A., Matthews, N., Gordon, L., Wetterstrand, H., DeClerck, F., Shah, M., Steduto, P., de Fraiture, C., Hatibu, N., Unver, O., Bird, J., Sibanda, L., and Smith, J. 2017. Sustainable intensification of agriculture for human prosperity and global sustainability. Ambio 46, 4–17. doi:10.1007/s13280-016-0793-6

Rosenzweig, C., Jones, J.W., Hatfield, J.L., Ruane, A.C., Boote, K.J., Thorburn, P., Antle, J.M., Nelson, G.C., Porter, C., Janssen, S., Asseng, S., Basso, B., Ewert, F., Wallach, D., Baigorria, G., and Winter, J.M. 2013. The Agricultural Model Intercomparison and Improvement Project (AgMIP): Protocols and pilot studies. Agric. For. Meteorol. 170, 166–182. doi:10.1016/j.agrformet.2012.09.011

Roy, P., Nei, D., Orikasa, T., Xu, Q., Okadome, H., Nakamura, N., and Shiina, T. 2009. A review of life cycle assessment (LCA) on some food products. J. Food Eng. 90, 1–10. doi:10.1016/j.jfoodeng.2008.06.016

Sándor, R. and Fodor, N. 2012. Simulation of soil temperature dynamics with models using different concepts. ScientificWorldJournal. 2012, 590287. doi:10.1100/2012/590287

Sau, F., Boote, K.J., Bostick, W.M.N., Jones, J.W., and Mínguez, M.I. 2004. Testing and improving evapotranspiration and soil water balance of the DSSAT crop models. Agron. J. 96, 1243–1257. doi:10.2134/agronj2004.1243

Schau, E.M. and Fet, A.M. 2008. LCA studies of food products as background for environmental product declarations. Int. J. Life Cycle Assess. 13, 255–264. doi:10.1065/lca2007.12.372

Sepulcre-Cantó, G., Gellens-Meulenberghs, F., Arboleda, A., Duveiller, G., De Wit, A., Eerens, H., Djaby, B., and Defourny, P. 2013. Estimating crop-specific evapotranspiration using remote-sensing imagery at various spatial resolutions for improving crop growth modelling. Int. J. Remote Sens. 34, 3274–3288. doi:10.1080/01431161.2012.716911

Shaffer, M.J., Lasnik, K., Ou, X., and Flynn, R. 2001a. NLEAP Internet Tools for estimating NO3-N leaching and N2O emissions. In: Shaffer, M.J., Ma, L., Hansen, S. (eds.), Modeling Carbon and Nitrogen Dynamics for Soil Management. Lewis publishers (CRC Press, LLC), Boca raton, Fl.

Shaffer, M.J., Ma, L., and Hansen, S. 2001b. Modeling carbon and nitrogen dynamics for soil management. Lewis Publishers, Boca Raton, Fla.

Sharpley, A.N. and Williams, J.R. 1990. EPIC — Erosion / Productivity Impact

Calculator: 1. Model documentation. Technical Bulletin 1768. U.S. Departement of Agriculture.

Šimůnek, J., M. Šejna, A., Saito, H., Sakai, M., and van Genuchten, M.T. 2013. The HYDRUS-1D Software Package for Simulating the Movement of Water, Heat, and Multiple Solutes in Variably Saturated Media. Version 4.17. Department of Environmental Sciences, University of California Riverside., Riverside, California.

Singh, J., Knapp, H.V., Arnold, J.G., and Demissie, M. 2005. HYDROLOGICAL MODELING OF THE IROQUOIS RIVER WATERSHED USING HSPF AND SWAT. J. Am. Water Resour. Assoc. 41, 343–360. doi:10.1111/j.1752-1688.2005.tb03740.x

Smith, J., Gottschalk, P., Bellarby, J., Richards, M., Nayak, D., Coleman, K., Hillier, J., Flynn, H., Wattenbach, M., Aitkenhead, M., Yeluripurti, J., Farmer, J., Smith, P., and Smith, J. 2010. Model to Estimate Carbon in Organic Soils – Sequestration and Emissions (ECOSSE). Carbon N. Y. 1–73.

Smith, P., Smith, J.U., Powlson, D.S., Mcgill, W.B., Arah, J.R.M., Chertov, O.G., Coleman, K., Franko, U., Frolking, S., Jenkinson, D.S., Jensen, L.S., Kelly, R.H., Klein-gunnewiek, H., Komarov, A.S., Li, C., Molina, J.A.E.J., Mueller, T., Parton, W.J., Thornley, J.H.M., and Whitmore, A.P. 1997. A comparison of the performance of nine soil organic matter models using datasets from seven long-term experiments. Geoderma 81, 153–225.

Sonesson, U., Berling, J., and Ziegler, F. 2010. Environmental assessment and management in the food industry. Life cycle assessment and related approaches. Woodhead Publishing Limited, UK.

Stasinopoulos, P., Compston, P., Newell, B., and Jones, H.M. 2012. A system dynamics approach in LCA to account for temporal effects—a consequential energy LCI of car body-in-whites. Int. J. Life Cycle Assess. 17, 199–207. doi:10.1007/s11367-011-0344-0

Stockle, C.O., Donatelli, M., and Nelson, R. 2003. CropSyst, a cropping systems simulation model. Eur. J. Agron. 18, 289–307. doi:Pii S1161-0301(02)00109-0

Suopajärvi, H.J. 2011. Sustainability Assessment: Principles, Frameworks, Indicators and Tools.

Tarboton, D.G. 2003. Rainfall - runoff processes. A workbook to accompany the Rainfall-Runoff Processes Web module. Civil and Environmental Engineering Faculty Publications. Utah State University.

The MathWorks Inc 2010. MATLAB.

Thorp, K., Barnes, E., and White, J.W. 2014. Evaluation of CSM-CROPGRO-Cotton for Simulating Effects of Management and Climate Change on Cotton Growth and Evapotranspiration in an Arid Environment. Trans. ASABE 1627–1642. doi:10.13031/trans.57.10612

Tsuji, G.., Hoogenboom, G., and Thornton, P.K. 1998. Understanding Options for Agricultural Production, Systems Approaches for Sustainable Agricultural

Development. Springer Netherlands, Dordrecht. doi:10.1007/978-94-017-3624-4
Tukker, A. and Jansen, B. 2006. Environmental Impacts of Products: A Detailed Review of Studies. J. Ind. Ecol. 10, 159–182. doi:10.1162/jiec.2006.10.3.159
Udo deHaes, H.A., Finnveden, G., Goedkoop, M., Hauschild, M., Hertwich, E.G., Hofstetter, P., Jolliet, O., Klopffer, W., Krewitt, W., Lindeijer, E., Mueller-Wenk, R., Olsen, S.I., Pennington, D.W., Potting, J., and Steen, B. 2002. Life cycle impact assessment: striving towars best practice. Society of Environmental Technology and Chemistry (SETAC), Pensacola.
United Nations 1987. Report of the World Commision on Environment and Development: Our Common Future - Brundtland Report. A/42/427. Oxford University Press.
USDA-NRCS 1986. Urban Hydrology for Small Watersheds. Technical Release 55. United States Departement of Agriculture - Natural Resource Conservation Service Conservation Engineering Division.
USDA-NRCS 2004. Estimation of Direct Runoff from Storm Rainfall. In: National Engineering Handbook Part 630 Hydrology. United States Department of Agriculture - Natural Resources Conservation Service. Washington.
Valdivia, S., Ugaya, C.M.L., and Sonnemann, G. 2013. LIFE CYCLE SUSTAINABILITY ASSESSMENT : FROM LCA TO LCSA A UNEP / SETAC approach towards a life cycle sustainability assessment — our contribution to Rio + 20 1673–1685. doi:10.1007/s11367-012-0529-1
Van Cauwenbergh, N., Biala, K., Bielders, C., Brouckaert, V., Franchois, L., Garcia Cidad, V., Hermy, M., Mathijs, E., Muys, B., Reijnders, J., Sauvenier, X., Valckx, J., Vanclooster, M., Van der Veken, B., Wauters, E., and Peeters, a. 2007. SAFE—A hierarchical framework for assessing the sustainability of agricultural systems. Agric. Ecosyst. Environ. 120, 229–242. doi:10.1016/j.agee.2006.09.006
Van Der Burgt, G.J.H.M., Oomen, G.J.M., Habets, A.S.J., and Rossing, W.A.H. 2006. The NDICEA model, a tool to improve nitrogen use efficiency in cropping systems. Nutr. Cycl. Agroecosystems 74, 275–294. doi:10.1007/s10705-006-9004-3
van Genuchten, M.T. 1980. A Closed-form Equation for Predicting the Hydraulic Conductivity of Unsaturated Soils1. Soil Sci. Soc. Am. J. 44, 892. doi:10.2136/sssaj1980.03615995004400050002x
Van Laar, H.H., Goudriaan, J., and Van Keulen, H. 1997. SUCROS97 : Simulation of crop growth for potential and water-limited production situations, as applied to spring wheat. AB-DLO, Wageningen.
Van Loon, J., Vansteenkiste, J., Diels, J., and Schrevens, E. 2011. Developing and testing a model for open field horticultural crops to enable use of a “just-in-time” fertilization management In: 19th International Congress on Modelling and Simulation (Modsim2011). Perth, Australia, pp. 1016–1022.

Van Steertegem, M. 2013. MIRA Indicator Report 2012. Flemish Environment Agency (VMM).
Vanclooster, M., Viaene, P., Christiaens, K., and Ducheyne, S. 1996. WAVE: a mathematical model for simulating water and agrochemicals in the soil and vadose environment. Refernce and user's manual (Release 2.1). Technical report. Institute for Land and WaterManagement, KU Leuven, Belgium.
Vansteenkiste, J., Van Loon, J., Garré, S., Pagès, L., Schrevens, E., and Diels, J. 2014. Estimating the parameters of a 3-D root distribution function from root observations with the trench profile method: case study with simulated and field-observed root data. Plant Soil 375, 75–88. doi:10.1007/s11104-013-1942-3
VDI 1997. Cumulative energy demand (KEA) - Terms, definitions, methods of calculation. VDI-Standard: VDI Richtlinien 4600. Verein Deutscher Ingenieure. Düsseldorf.
VLM 2008. Analyse van Nitraatstikstofresidumetingen in de tuinbouw. Eindrapport. VLM/MESTBANK/TWOL2006/MB2006/4. Bodemkundige Dienst van België vzw i.s.m. Universiteit Gent, Vakgroepbeheer en bodemhygiëne (UGBB) in opdracht van de Vlaamse Landmaatschappij Afdeling Mestbank.
VLM 2015. Actieprogramma ter uitvoering van de nitraatrichtlijn 2015-2018. Vlaamse landmaatschappij (VLM).
VLM 2017. Normen en richtwaarden 2017. Vlaamse Land Maatschappij (VLM).
VMM 2016. Nutriënten in oppervlaktewater in landbouwgebied, resultaten MAP-meetnet 2015-2016.
Vogeler, I., Giltrap, D., and Cichota, R. 2012. Comparison of APSIM and DNDC simulations of nitrogen transformations and N2O emissions. Sci. Total Environ. doi:10.1016/j.scitotenv.2012.09.021
von Hoyningen-Huene, J. 1984. Die Interzeption des Niederschlags in landwirtschaftlichen Pflanzenbeständen. In: Kulturbau, D. verband für wasserwirtschaft und (ed.), DVWK Schriften 57 - EinfluB Der Landnutzung Auf Den Gebietswasserhaushalt. Hamburg, pp. 1–53.
Wallach, D., Makowski, D., Jones, J.W., and Brun, F. 2014. Working wih dynamic crop models. Methods, tools and examples for agriculture and environment. Second Edition. Elsevier. doi:doi.org/10.1016/C2011-0-06987-9
Wang-erlandsson, L. 2014. Contrasting roles of interception and transpiration in the hydrological cycle – Part 1 : Simple Terrestrial Evaporation to Atmosphere Model 203–279. doi:10.5194/esdd-5-203-2014
Wei, Y., Davidson, B., Chen, D., and White, R. 2009. Agriculture , Ecosystems and Environment Balancing the economic , social and environmental dimensions of agro-ecosystems : An integrated modeling approach 131, 263–273. doi:10.1016/j.agee.2009.01.021
Williams, A.G., Audsley, E., and Sandars, D.L. 2006. Determining the environmental burdens and resources use in the production of agricultural

and horticultural commodities. Main report. Defra research project ISO205.
Williams, A.G., Audsley, E., and Sandars, D.L. 2010. Environmental burdens of producing bread wheat , oilseed rape and potatoes in England and Wales using simulation and system modelling 855–868. doi:10.1007/s11367-010-0212-3
Williams, J.R., Renard, K.G., and Dyke, P.T. 1983. EPIC - A new method for assessing erosion’s effect on soil productivity. J. Soil Water Conserv. 38, 391–383.
Willmott, C.J. 1981. On the validation of models. Phys. Geogr. 2, 184–194. doi:10.1080/02723646.1981.10642213
Woodward, D.E., Hawkins, R.H., Jiang, R., Hjelmfelt, Jr., A.T., Van Mullem, J.A., and Quan, Q.D. 2003. Runoff Curve Number Method: Examination of the Initial Abstraction Ratio In: World Water & Environmental Resources Congress 2003. American Society of Civil Engineers, Reston, VA, pp. 1–10. doi:10.1061/40685(2003)308
Zekki, H., Gary, C., Gosselin, A., and Gauthier, L. 1999. Validation of a Photosynthesis Model through the Use of the CO2Balance of a Greenhouse Tomato Canopy. Ann. Bot. 84, 591–598. doi:10.1006/anbo.1999.0938
Zhang, J. 2010. Temperature sensitivity of soil organic matter decomposition and the influence of soil carbon pools and attributes. PhD dissertation. Iowa State University, Ames, Iowa.
Zhang, X., Davidson, E.A., Mauzerall, D.L., Searchinger, T.D., Dumas, P., and Shen, Y. 2015. Managing nitrogen for sustainable development. Nature 1–9. doi:10.1038/nature15743
Zimmermann, M., Leifeld, J., Schmidt, M.W.I., Smith, P., and Fuhrer, J. 2007. Measured soil organic matter fractions can be related to pools in the RothC model. Eur. J. Soil Sci. 58, 658–667. doi:10.1111/j.1365-2389.2006.00855.x

Schrevens E., Heuts, R.F. and Diels, J. Potential strategies to reduce nitrogen emissions to the environment in an intensive cauliflower-leek rotation system: a modelling approach (2018). Acta Hortic. XXX. The International Horticultural Congress. IHC 2018. Istanbul, Turkey. (accepted for oral presentation)

Heuts R.F., Vansteenkiste J., Diels J., Schrevens E. Model based life cycle assessment of nitrogen fertilization in a cauliflower-leek rotation system (2016). Acta Hortic. 1112, 403-410. The 29th International Horticultural Congress. IHC2014 Brisbane,Australia (ISHS). doi: 10.17660/ActaHortic.2016.1112.54

Grados, D., Heuts, R.F., Vetters, E., Schrevens, E. A model based comprehensive analysis of technical sustainability of potato production systems in the Mantaro Valley, Central Highlands, Peru (2016). 5th International Symposium on Applications of Modelling as an Innovative Technology in the Horticultural Supply Chain – Model-IT 2015, Wageningen, The Netherlands (ISHS).

Almeida, J., Achten, W. M.J., Verbist, B., Heuts, R. F., Schrevens, E. and Muys, B. Carbon and Water Footprints and Energy Use of Greenhouse Tomato Production in Northern Italy (2014). Journal of Industrial Ecology, 18 (6):898–908. doi: 10.1111/jiec.12169

Heuts R.F., Van Loon J., Schrevens E. Life cycle assessment of different heating systems for glasshouse tomato production in Flanders, Belgium (2012). Acta Hort. (ISHS) 957:107-114, 4th symposium on models for planth growth, environmental control and farm management in protected cultivation, Hortimodel 2012; Doi: 10.17660/ActaHortic.2012.957.11

Van Loon J., Heuts R.F., Vansteenkiste J., Diels J., Schrevens E. Uncertainty of Decision support systems in Horticultural production. Impact on accuracy from a fully monitored to a minimal data framework (2012). Acta Hort. (ISHS) 957:281-288, 4th symposium on models for plant growth, environmental control and farm management in protected cultivation, Hortimodel 2012; http://www.actahort.org/books/957/957_32.htm

Vansteenkiste J., Van Loon J., Heuts R.F., Schrevens E., Diels J. Nitrogen uptake in field vegetable production: modelling broadcast and row application (2012). Acta Hort. (ISHS) 957:115-122, 4th symposium on models for plant growth, environmental control and farm management in protected cultivation, Hortimodel 2012; http://www.actahort.org/books/957/957_12.htm

Heuts R.F., Van Loon J., Schrevens E. Life cycle assessment of various fertilization treatments in open field vegetable production, Flanders, Belgium (2012). *The 8th International Conference on LCA in the Agri-Food Sector*, Saint-Malo, France, 2-4 okt 2012 (poster presentation)

Heuts R.F., Van Loon J., Schrevens E. Investigating the probability distribution between global warming and acidification of the pesticide management in greenhouse tomato production: a regional LCA for the Boyacá department, Colombia (2012). *LCA XII conference*, The Amercian Center for Life Cycle Assessment (ACLCA), Tacoma, Washington, 25-27 sept 2012 (oral presentation)