AMERICAN UNIVERSITY OF BEIRUT

INCORPORATING NITROGEN IN THE WATER-ENERGY-FOOD NEXUS: AN OPTIMIZATION APPROACH

by
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AN ABSTRACT OF THE THESIS OF

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Growing populations and improved standards of living are spiking the global demands for food. Coping with this challenge, agricultural systems casted unprecedented stress on water, land, and nutrient cycling at all scales. Of those nutrients, nitrogen quickly evolved as a major limiting factor for plant growth up until the discovery of the Haber-Bosch process, which made reactive nitrogen available at an industrial scale. This facilitated intensified agriculture, thus boosting the efficiency of agricultural systems and leading to yields that traditional agricultural practices could not deliver. Unfortunately, this translated into intensified application of nitrogen fertilizers to meet the growing crop yield targets in food production, resulting in excessive reactive nitrogen entering our ecosystem causing detrimental effects on the environment and human health, as well as threatening Earth's resilience. Furthermore, reactive nitrogen production is energy-intensive and generates a substantial energy and carbon footprint. This calls for the development of holistic nitrogen management approaches to limit nitrogen's adverse effects. In this study, we develop a mathematical optimization model for the optimal application of nitrogen to meet an evolving and growing agricultural agenda, under a water-energy-food nexus framework. The model optimizes for nitrogen allocation under sustainable water, food and energy security targets, where the nitrogen planetary boundary is the primary environmental constraint, in addition to other nutritional, socio-economic and natural resources constraints. We attempt to optimize the nitrogen footprint required to meet current and future food demands, taking water, energy and carbon footprints into account as well. We incorporate the nitrogen cycle within the land-crop-food continuum and utilize nitrogen use efficiency as a primary indicator. The model serves as a decision-making tool for optimum nitrogen application based on nitrogen demands from optimized agricultural policy. It reallocates different nitrogen sources (industrial, natural, or recycled) available at the regional scale into the farm scale. The model is validated using a hypothetical case study to test the sensitivity of the nexus to nitrogen input and nitrogen use efficiency, under several resource availability scenarios and different policy targets.

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CHAPTER I

INTRODUCTION

Nitrogen (N) plays an indispensable role in food security as a limiting nutrient for crop growth. Despite its abundance, it is not readily available to us (Galloway et al., 2003). 99% of the nitrogen on Earth is unreactive, present in the form of dinitrogen N_2 gas (IFA, 2010). It can naturally be transformed to reactive or reduced nitrogen Nr (NH_3, NH_4^+, NO_3^-, NO_x, N_2O …) either by lightning or by biological nitrogen fixation, a process exclusive to a specific type of nitrogen fixating organisms. Industrial fixation of nitrogen only became possible after the development of the Haber-Bosch process in 1909, which produces ammonia NH_3 from its elements (Stein and Klotz, 2016). This paved the way to commercially available synthetic nitrogen fertilizers in the 1950's (International Fertilizer Industry Association and United Nations Environment Programme, 2002; US EPA, 2008; Widdison and Burt, 2008). As a result, intensified agriculture became feasible, resulting in higher input of fertilizers necessary for increased crop yields and increased profit.

To cope with growing populations and meet increasing food demands, reliance on synthetic nitrogen fertilizers has increased exponentially to the point where it now provides food for 2 out of every 5 persons (Smil, 2001). Unfortunately, this has disrupted the natural nitrogen cycle and the ecosystem processes that rely on its balance, and has caused environmental drawbacks from excessive inputs of reactive nitrogen into our ecosystems. Currently, over 50% of total reactive nitrogen on Earth is of anthropogenic origin and 63% of that is due to nitrogenous fertilizers alone (Dobermann, 2005). Application of nitrogenous fertilizers in agriculture resulted in increased rates of ammonia volatilization and higher nitrous oxide (N_2O) emissions, both contributing to climate change. Nitrogen fertilizers are also responsible for excessive leaching of nitrates (NO_3^-) and nitrites (NO_2^-) to water bodies, causing algal blooms, eutrophication, and in extreme situations, development of "dead zones". Aside from agriculture, nitrogen is a primary polluting by-product of the energy and transport industries, with N_2O and NO_x emitted with fossil fuel combustion acting as greenhouse gases (GHGs) contributing to the ozone depletion and global warming.

From the above, we come to two main observations. The first observation is the evolution of the effects of excessive reactive nitrogen input from a local scale to a global one (Galloway et al., 2003). It is what makes the nitrogen biogeochemical cycle an "aggregated" process; which means that in addition to their direct effect on immediate ecosystems, nitrogen compounds also pose a threat to the environment's resilience as a whole (Sutton and UNEP, 2013). This was highlighted in 2009 when the planetary boundaries concept was first introduced. The biogeochemical cycles of nitrogen and phosphorus were recognized as planetary boundaries, and research showed that their thresholds had already been exceeded (Rockström et al., 2009; Steffen et al., 2015) (Figure 1). The second observation is that nitrogen is linked to all three sectors of water, energy and food. Nitrogen's ability to boost agricultural yields makes it integral to food security, its being a component of fossil fuels and a requirement for biofuel production means it is indispensable to energy security, and its polluting effect ties it well with water security and climate change. This also imposes that any management on the nutrient level takes into consideration the mutual effect that nitrogen shares with the sectors, which are highly interlinked themselves. This interlinkage can be best illustrated by adopting a Water-Energy-Food Nexus (WEF nexus) framework. First introduced in 2008 at the World Economic Forum and established in 2011 at the Bonn Conference, the nexus describes the interdependencies of the different sectors with an aim of ensuring the security of each (Hoff, 2011). Adding nitrogen as a fourth pillar can be a way to evaluate the relations between nitrogen and the WEF, enabling the optimal use of each to meet specific policy targets.

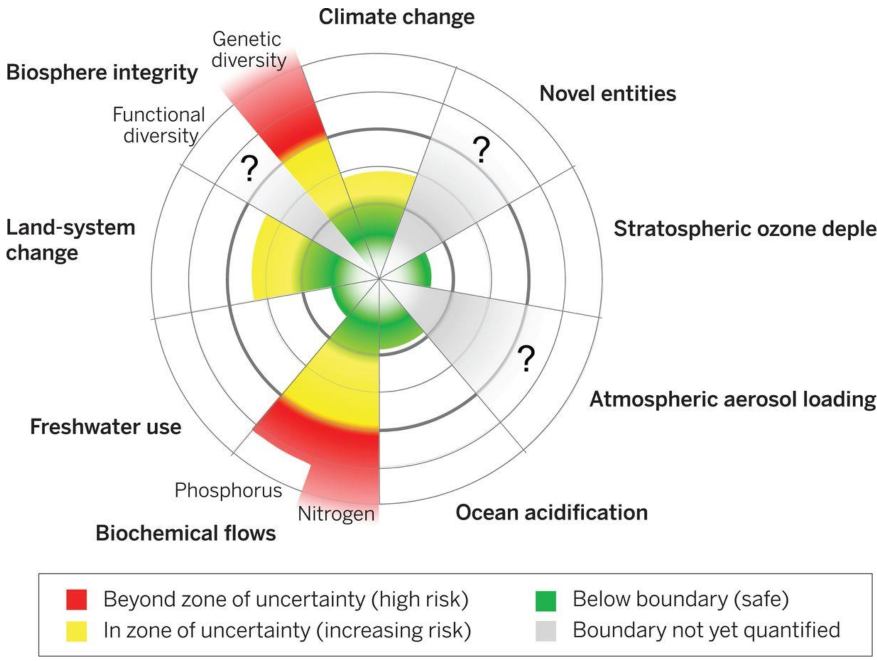


Figure 1: The planetary boundaries, from Steffen et al. (2015)

Since 2011, the nexus has appeared in the literature as an emerging framework for resource use and alleviation of environmental impacts. Application of the nexus followed different methodologies including physical models (Daher and Mohtar, 2015; Tian et al., 2018), cost benefit analysis (Endo et al., 2015), life cycle assessment (Al-Ansari et al., 2015; Yuan et al., 2018), and material flow analysis (Biggs et al., 2015). Out of the different approaches, optimization stands out as an efficient methodology for resource allocation as it harnesses synergies and connects different and competing components of the problem understudy (Endo et al., 2015). Yet, the WEF nexus is a large multi-sector, multi-scale resource allocation problem whose optimization is still a relatively open field of research. Few exceptions include Karan et al. (2018) who maximized sustainability at a greenhouse scale by optimizing its design elements to meet the demands of a household of four persons. Uen et al. (2018) maximized WEF benefits (water shortage reductions, hydropower production, and food production) at a reservoir scale by dynamic multi-objective optimization of the operations of the Shihmen Reservoir. More examples were observed at the national scale with models like the WEF Optimization (WEFO) model developed by Zhang and Vesselinov (2017), and the WEF Nexus Index (WEFNI) for crops introduced by El-Gafy (2017), both aiming to maximize economic water, energy and food production, constrained by demands, available resources, and environmental boundaries. Other studies added further constraints and couplings that extend the nexus to cover the effects of climate, nutrients, consumption behaviour and different economic policies into the model formulation (Bieber et al., 2018; Leung Pah Hang et al., 2016; Smajgl et al., 2016). Out of the few who took nutrients into consideration are Liu et al. (2016) and Conijn et al. (2018). Liu et al. (2016) studied nitrogen flows on a global scale, including those of nitrogen embedded in trade. They aimed to assess nitrogen’s role in meeting the hunger eradication targets set by the Millennium Development Goals. Conijn et al. (2018) presented a similar approach but set the planetary boundaries as the primary constraint. Their developed model, BIOSPACS, simulated nitrogen and phosphorus flows in the food system, and quantified industrial and intended biological fixation of nitrogen, energy imbalance at the top of the atmosphere, and change in area of forested land due to agriculture. Both studies assess different diet shift, nitrogen use, and reduced waste scenarios, and conclude that combined efforts of technology, policies, and consumption trends are necessary for humans to have a chance at reversing the consequences of expanding agriculture on the environment while meeting food security targets.

Recognizing the need for an explicit coupling between the cycling of major biogeochemical elements (particularly nitrogen, carbon and phosphorous) and the nexus, we present an optimization model that establishes the relations between nitrogen and the Water-Energy-Food nexus. We build on the water-food model developed by Mortada et al. (2018) by incorporating the nitrogen cycle into the generalized model, setting the nitrogen fixation planetary boundary as a main constraint, and using Nitrogen Use Efficiency as a primary indicator. The model takes available natural resources and national water, food and energy demands to give the optimal nitrogen use and resource allocation per specific objective functions and under different scenarios (Figure 2). Being multi-scale, it allows for nutrient tracing and management from farm to global scales. Guided by water, energy and food security targets, the model capitalizes on the strong correlation between nitrogen management measures and the WEF nexus to address local and global concerns including the following: (1) How do policy decisions vary when targeting a high nitrogen use efficiency versus a low nitrogen input? (2) How can policies targeting behavioural dietary changes or resource management improve nitrogen efficiencies in meeting WEF nexus demands? And (3) To what extent can we sustain self-sufficiency under nitrogen planetary boundary limits? The model was validated by a hypothetical case study demonstrating the model's abilities to response to specific objective functions and varying resource constraints.

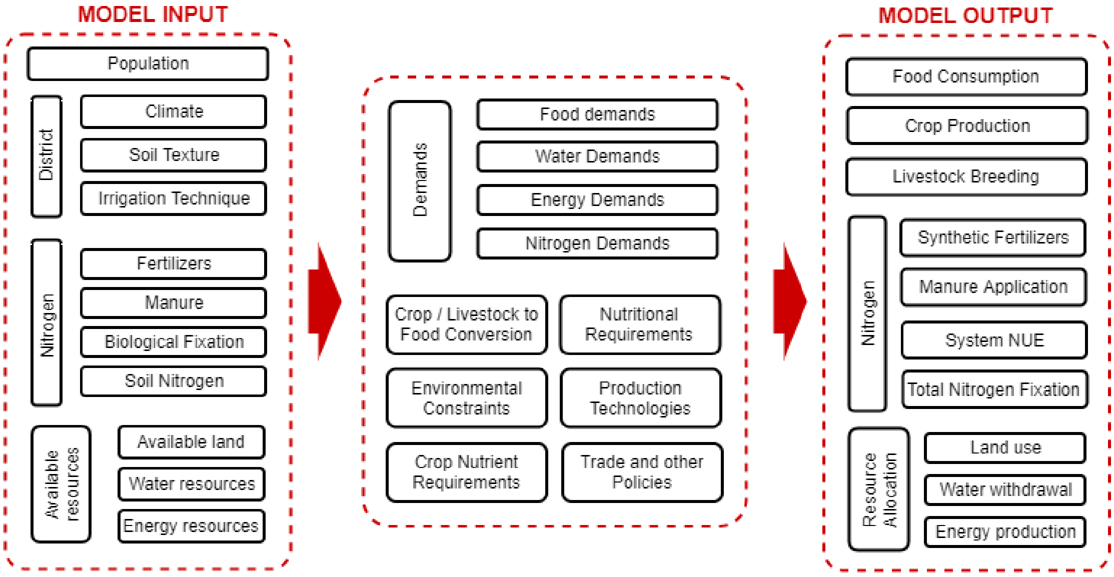


Figure 2: The broad model framework

CHAPTER II

BACKGROUND ON NITROGEN

The model attempts to formulate the most significant nitrogen flows having direct effect on the natural nitrogen cycle, how anthropogenic activities have altered it, and its overall effect on the environment. Therefore, it is important to have a good understanding of the natural nitrogen cycle and its driving factors. In this section, we present the terrestrial nitrogen cycle, quantify nitrogen relations with the water, energy and food sectors, and define the primary indicator used in this thesis: Nitrogen Use Efficiency.

A. The Terrestrial Nitrogen Cycle

Nitrogen is present in the global ecosystem in three different forms: atmospheric nitrogen (N_2), organic nitrogen from the decomposition of litter fall and animal excretions, and inorganic nitrogen (ammonium NH_4^+ and nitrates NO_3^-). Nitrogen cycles through these different forms between land, water and the atmosphere via several physical and microbial processes. Atmospheric nitrogen is first transferred to land and water bodies by dry or wet deposition, adding to the pool of inorganic nitrogen through its dissolution. Plants take up this nitrogen from the soil to build their biomass and transform it to proteins, and animals get a hold of it through eating those plants. Withering of plants and animal excretions returns part of that nitrogen to the soil in organic form, which is then transformed to inorganic form by mineralization and nitrification due to special microbes called rhizobia. Inorganic nitrogen is returned back to the atmosphere as N_2 or N_2O through another microbial process called denitrification, and that closes the cycle (Davidson et al., 2016; Lin et al., 2000) (Figure 3).

Plants have two main sources of nitrogen: the atmospheric nitrogen directly fixed through biological nitrogen fixation (BNF), and inorganic soil nitrogen fixed through its roots. Biological nitrogen fixation, or the process that allows the plant to take inert N_2 from the air and “fix” it, transform it to ammonia NH_3, is only possible for legumes. Other plants use the inorganic nitrogen soluble in the soil or irrigation water. However, not all present nitrogen is available for plant uptake. Nitrogen in the soil is always under transformation and is prone to being lost through: ammonia volatilization by ammonification from the organic pool, nitrate leaching to surface and ground water, or emission of gaseous nitrogen during the nitrification process. These losses compromise plants growth and call for the need for additional nitrogen to make up for that lost, thus leading to reduction in nitrogen use efficiency.

The main disruption to the nitrogen cycle came with the application of synthetic fertilizers and fossil fuel combustion. Both added to the reactive nitrogen input to Earth’s ecosystems, as they are forms of nitrogen fixation, and resulted in higher loss rates. The consequence was accumulation of reactive nitrogen at specific locations in amounts beyond what the natural ecosystem could accommodate for, resulting in the detrimental effects of increased N_2O and NH_3 emissions or nitrate leaching (Galloway et al., 2003; Reay, 2015).

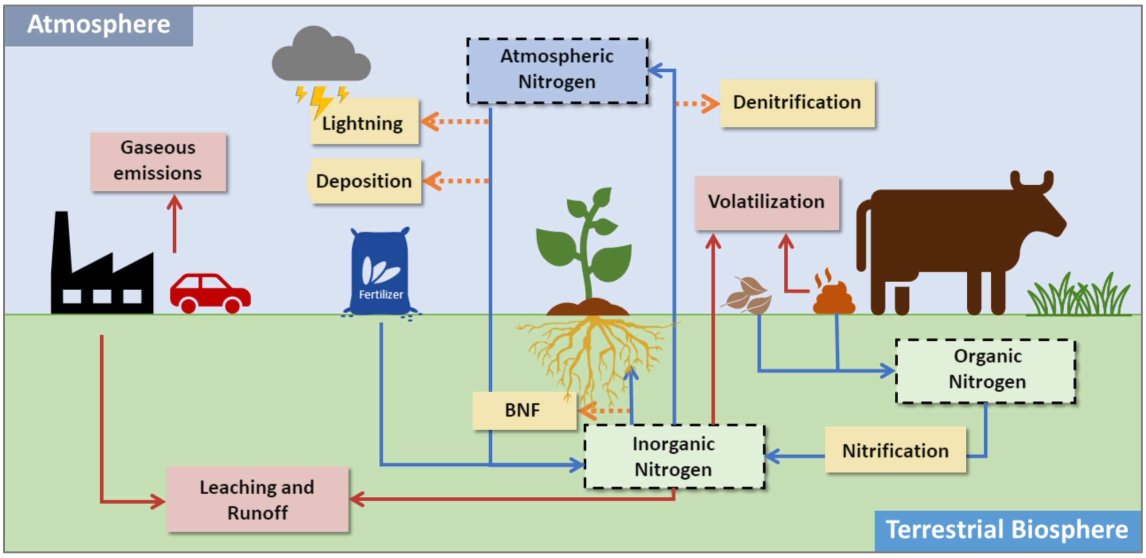


Figure 3: The terrestrial nitrogen cycle and the anthropogenic contribution.

B. Nitrogen and the Nexus

Nitrogen is a vital contributor to the water-energy-food nexus, as it acts as a factor affecting all three sectors. It is important to identify the respective nitrogen flow to each sector as well as the contribution of each sector to global nitrogen fixation (reactive nitrogen). Those links are described as follows:

1. Nitrogen and Food

Whether through nitrogen requirements for crop production, which is our primary focus, or through food protein nutritional demands, this relation proves indispensable to describe the food security status. Croplands receive around 136 TgN each year, half of which is provided from synthetic nitrogen fertilizers alone, while only 16% comes from biological nitrogen fixation. 55% of total nitrogen input to croplands is removed with harvested crops each year (Liu et al., 2010; Smil, 1999).

2. Nitrogen and Water

Available soil nitrogen and nitrate runoff rates are highly linked to soil water content as well as irrigation techniques used. Moreover, excessive fertilizer input in agricultural lands has been the main driver of algal blooms and eutrophication worldwide. Almost 30% of input nitrogen is lost through nitrate leaching to downstream water bodies (IPCC, 2006a). Furthermore, water bodies act as nitrogen sinks fixing more than half of total global annual nitrogen, accounting to 140 TgN/year (Smil, 1999).

3. Nitrogen and Energy

Fertilizer production is an energy intensive process with high energy footprint (using 1.2% of total global energy production). The Haber-Bosch process alone produces 120 TgN/yr of nitrogen for both fertilizer and industrial chemical use. On the other hand, fossil fuel combustion, which is a form of anthropogenic nitrogen fixation, is a major source of nitrogenous compounds emissions, emitting 30 TgN yearly into the atmosphere (Fowler et al., 2013). Our model accounts for those relations through quantifying nitrogen demand for crop production, nitrate leaching and ammonia emissions from agriculture, as well as nitrogen emissions from energy production processes.

C. Nitrogen Use Efficiency

In simple terms, nitrogen use efficiency (NUE) is a ratio of nitrogen outputs to nitrogen inputs. It represents how much nitrogen is recovered in the crop biomass versus the nitrogen supply available to it (Cassman et al., 2002). However, the term is so broad that it allows to assess nitrogen use at different scales, based on various nitrogen budgets, and in several agricultural systems (Dobermann, 2005). NUE is an indication of the efficiency of the overall cropping system; which is a function of crop management (tillage, rotation, irrigation, drainage, crop covering..), fertilizer management (rate, timing, placement..), as well as weather and soil properties (Gregorich et al., 2015). On average, NUE is the lowest in dairy grazing systems (0.15 - 0.35) with high nitrogen losses, and the highest (0.4 - 0.7) in ecological low-input systems. Unfortunately, while the latter systems generate lower nitrogen losses, they also generate lower yields (Spiertz, 2009).

Table 1 summarizes the several forms or variations that nitrogen use efficiency allows for. In Figure 4, we attempt to illustrate the soil-farm-land nitrogen budgets of Leip et al. (2011) mentioned in Table 1, noting their corresponding equations. At an agronomic level, nitrogen use efficiency is studied to evaluate crop N uptake efficiency. It is a small-scale indicator of N efficiency, usually assessed in a controlled environment of a plot, and over a specific time period. Applications of these N efficiencies aim at maximizing nutrient uptake and enhancing the microbial processes in the soil, as well as studying different factors that affect yield variations, and evaluating nitrogen management experiments. At a larger scale, evaluating nitrogen use efficiency aims at optimizing nutrient use and resource allocation. For that purpose, the second category of NUE’s would be more representative for a larger, more robust system, especially that it allows studying N stock variations along several cropping seasons or years, and could act as a guide to agricultural policy decisions (Dobermann, 2005; Pathak et al., 2011; Zhang et al., 2012, 2017).

Table 1: Definitions of nitrogen use efficiency in the literature

Approach	*Definition*	*Expression*	*Unit*	*Scale of Application*	*References*
Agronomic level	Partial Factor Productivity PFP$_N$	product yield / fertilizer application rate	kg.ha^{-1}/ kgN.ha^{-1}	Steady State Short Term: (up to one cropping season)	(Cassman et al., 2002; Dobermann, 2005; Spiertz, 2009)
	Agronomic N efficiency AE$_N$	crop yield increase*/ fertilizer application rate	kg.ha^{-1}/ kgN.ha^{-1}		
	Crop Recovery Efficiency of applied N RE$_N$	Increase* in N uptake/ fertilizer application rate	kgN.ha^{-1}/ kgN.ha^{-1}		
	Physiological Efficiency of applied N PE$_N$	crop yield increase / increase in N uptake	kg.ha^{-1}/ kgN.ha^{-1}		
	Apparent N Use Efficiency ANUE	N in grain / fertilizer application rate	kgN.ha^{-1}/ kgN.ha^{-1}		
System Boundary level	Soil	Equation (a)	kgN.ha^{-1}/ kgN.ha^{-1}	Steady/ Transient State Long Term: (One cropping season to several years)	(Leip et al., 2011) (Eurostat, 2013)
	Land	Equation (b)	kgN.ha^{-1}/ kgN.ha^{-1}		
	Farm-gate	Equation (c)	kgN.ha^{-1}/ kgN.ha^{-1}		
	System Nitrogen Efficiency SyNE	Equation (d)	kgN.ha^{-1}/ kgN.ha^{-1}		(Carof and Godinot, 2018; Godinot et al., 2014, 2015)
	Potential System Efficiency**	Net outputs / External system inputs	kgN.ha^{-1}/ kgN.ha^{-1}		
	Relative Nitrogen Efficiency RNE	SyNE / Potential Efficiency	kgN.ha^{-1}/ kgN.ha^{-1}		

Equation (a): NUE$_{soil}$ = (harvested crops + fodder crops + crop residues + soil N stock changes)/ (mineral fertilizers + manure applied + organic N sources + crop residues returned to/left on soil + BNF + atmospheric deposition)

Equation (b): NUE$_{land}$ = (harvested crops + fodder crops + crop residues)/ (mineral fertilizers + organic N sources + net manure import/export and withdrawal + manure excretion + crop residues returned to/left on soil + BNF + atmospheric deposition)

Equation (c): NUE$_{farm}$ = (harvested crops + animal products)/ (mineral fertilizers + net manure import/export and withdrawal + feed + organic N sources + BNF + atmospheric deposition)

Equation (d): SyNE = (harvested crops + animal products + manure excretion)/ [(livestock + mineral fertilizers + manure applied + feed + BNF + non-symbiotic fixation + atmospheric deposition + seeds + fuel) + (losses from inputs) - (change in N soil stock)]

* Any ”increase” in yield or N uptake refers to the obtained yield or N uptake achieved at the specified fertilizer application rate compared to a zero-fertilizer scenario

**Potential system efficiency is “ the best efficiency that can be attained in optimal conditions” (Godinot et al., 2015), where input losses are minimal and recycling is highest, obtained from the literature

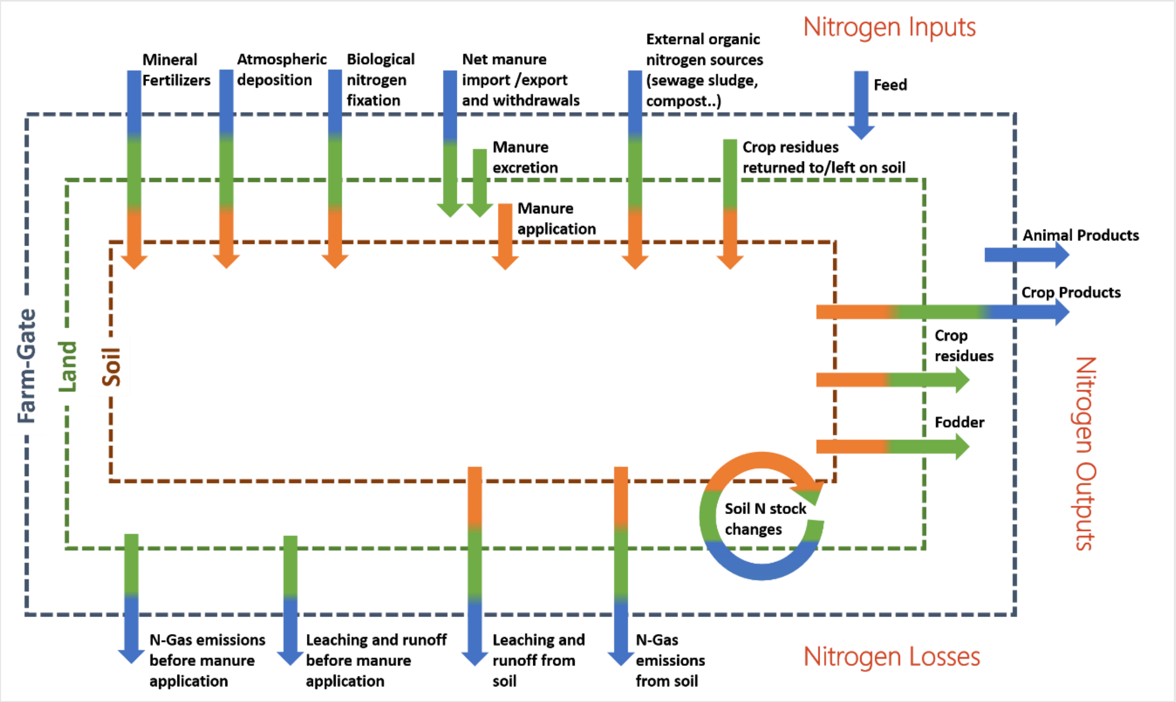


Figure 4: Illustration of Farm, Land, Soil nitrogen budgets from Leip et al. (2011)

As nitrogen's effects on the environment clashes with its critical role in providing food security, nitrogen management gets wide attention in research. Currently, this research works in parallel with both NUE levels and is focused around two approaches: 1) optimizing nitrogen use efficiency at the crop and soil agronomic level and ultimately maximizing crop yields, and 2) modelling nitrogen cycling and assessing nitrogen balance at a wider level, regional or global, for policy making purposes.

In the first approach, research is based on integrated nutrient management (INM) which studies root zone conditions and nutrient availability in order to manage fertilizer application following a "right amount, in the right place, at the right time" basis (Oenema and Pietrzak, 2002). Nutrient management models focus on achieving increased synchrony between nutrient supply and demand, by studying crop nutrient uptake under different climatic and soil conditions (Zhang et al., 2012). Cassman et al. (2002) introduced an expression for this synchrony relating fertilizer input to soil indigenous nitrogen and crop nitrogen uptake. By setting it against crop fertilizer uptake, they were able to notice a higher fertilizer efficiency for lower indigenous nitrogen, explained by N being a limiting nutrient in this case. Conversely, when nitrogen in the soil is abundant, fertilizer efficiency would decrease, calling for lower fertilizer application. Their results favour the recycling of available soil nitrogen. Drinkwater and Snapp (2007) took a similar approach but introduced an ecosystem framework to nutrient management. They argued that it is not enough to only reduce reliance on inorganic and soluble N, since with crop yields remaining the same at the beginning, the soil nitrogen pool will gradually decrease, deplete the soil, and eventually lead to lower yields. Therefore, their approach focused on promoting soil nutrient supply through microbial processes in parallel with increasing organic N pools and decreasing reliance on inorganic nitrogen.

In the second approach, INM studies were extended to show the effect on policy-making, how nitrogen management falls into general resource allocation decisions, and how to assess and compare different farming systems. Research focuses on modelling nutrient cycling and assessing nitrogen budgets, in order to monitor spatial and temporal variations of the N balance, as well as examine policy effects on N input and emissions (de Vries et al., 2011). Leip et al. (2011) focused on the different system boundaries that define the nitrogen budget or the nitrogen use efficiency. They presented three systems: farm, land, and soil; and compared them in terms of their accounting for certain factors, such as animal products, feed, crop residues, soil N stock variation, N emissions and nitrate leaching.

Godinot et al. (2014, 2015) introduced two new indicators that improve on basic farm NUE: System Nitrogen Efficiency (SyNE) and Relative Nitrogen Efficiency (RNE). They argued that the former better depicts agricultural productivity of a farming system than the conventional farm-gate NUE since it accounts for all sources of nitrogen on a farm and their respective production nitrogen footprints through a life cycle assessment approach, which NUE traditionally doesn’t do. RNE, on the other hand, is an indicator that allows comparing the efficiencies of different farming systems, which also isn’t possible using NUE. In addition, they formulated a user-friendly tool that aids at calculating the developed indicators on a farm or regional level, consequently assisting in better assessment of the system understudy (Carof and Godinot, 2018).

D. Nitrogen Use Efficiency in our Model

The scale flexibility of our model allows us to evaluate NUE at different levels. The model also allows for agronomic efficiencies to be assessed at a crop level, such as PFP_N and ANUE. We primarily study NUE based on the soil level for every crop. We also compute NUE based on a farm-gate budget, which adds livestock nitrogen intake and animal product outputs into consideration. Nitrogen efficiency can also be studied at the global level accounting for import and export of goods as well, or nitrogen trade, which paves the way for virtual nitrogen assessment.

At the soil level, the main natural nitrogen inputs are biological nitrogen fixation and atmospheric deposition. We add to that the nitrogen available in soil, as well as the added agricultural inputs of nitrogen: synthetic fertilizers and applied manure. N output on the other hand is the nitrogen content removed with yielded crops, which in our calculations, accounts for harvested crops as well as fodder and grazing crops. Since we are working in a steady state, and on a span of one year or one cropping season, we're not accounting for any soil N changes, and crop residues are accounted for as lost N. In addition to that, nitrogen not taken up by the plant can be lost either through denitrification and gaseous emissions (N_2, N_2O, NO), ammonia volatilization, and nitrate leaching. To move from a soil to a farm budget, we add the livestock components, feed intake as input and animal products as output. Excreted nitrogen from livestock is used to calculate locally available manure. The adopted farm budget is illustrated in Figure 5.

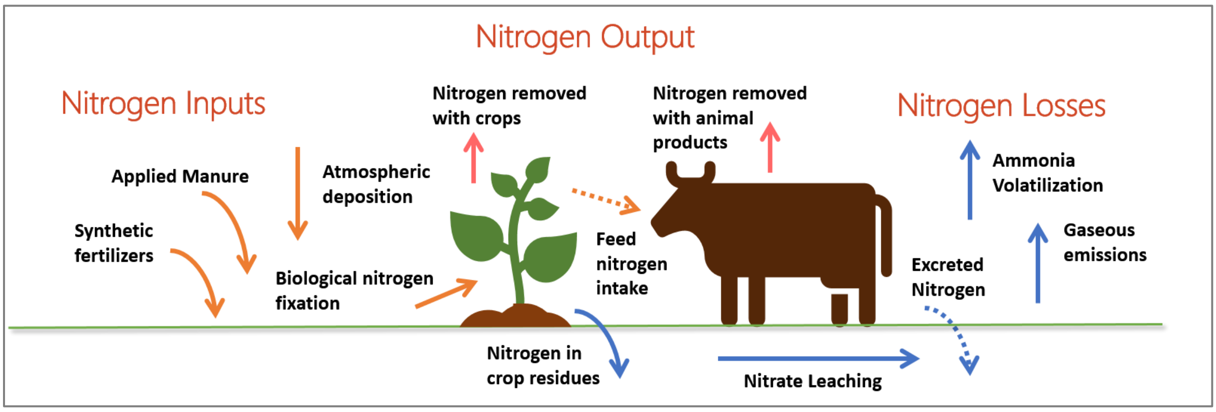


Figure 5: Nitrogen budget components adopted in the model

CHAPTER III
MODEL FORMULATION

A. Model Components

1. Food Items

We use the term “food items” to represent any food product of plant or animal origin, resulting from processing of crops or animal meat or dairy, and characterized by a set of nutrients. Food items are denoted by (i, j), where i stands for the food group and j for the item belonging to group i. Data on food groups and items were obtained from FAOSTAT.

2. Crops

Crops are cultivated plants grown to meet a certain demand for food production. In our model, we denote crops by (m, n), where m stands for the crop group and n for the crop belonging to group m. Crop classification and data were based on FAOSTAT.

3. Livestock and Feed

Mortada et al. (2018) implicitly accounted for the livestock sector in their model, by calculating the demand for fodder crops and animal product consumption. We realized the need for explicitly accounting for this sector due to its significant contribution to the nitrogen and carbon cycles. For that, we treat livestock as a new but similar category to crops. Livestock unit (m', n') stands for the animal type n' belonging to livestock group m'. This allows us to account for livestock production, export, import (live animal trade), as well as demand of livestock for meat and dairy production, and demand of feed for livestock. Similarly, in addition to food items (i, j), we accounted for feed items denoted by (i', j') to facilitate the calculation of cereal and fodder crop demands. It also allows us to account for feed consumption and demand, in addition to feed production, import and export. Data for livestock and feed were obtained from FAOSTAT.

4. Nitrogen

Based on a farm-gate balance and the natural processes that govern the nitrogen cycle, we account for the following nitrogen inputs, outputs, and losses:

a. Inputs

Nitrogen inputs are represented by all available nitrogen sources for the crop. Natural nitrogen inputs accounted for are Atmospheric Deposition $(NDEP)$ which is nitrogen deposited on land either dry or wet, Biological Nitrogen Fixation (BNF) which is the nitrogen fixation process known to legumes and specific crops, and Non-Symbiotic Fixation (NSF) that happens by free living organisms in the soil.

Added sources could either be from synthetic fertilizers (D_N_{FER}), or from animal manure (D_N_{MAN}).

b. Outputs

Nitrogen output is the nitrogen removed with the crop harvest calculated as the nitrogen content of the produced crops, as well as nitrogen available in animal products such as meat and dairy.

c. Losses

Losses in our model represent all products of nitrogen inputs that were not taken up by the crop. These nitrogen losses take different forms. We account for nitrogen lost through denitrification ($NGAS$), nitrate leaching ($NLEACH$), and ammonia volatilization ($NVOL$). Adopted emission and leaching factors are presented in Table 16 of Appendix B: Data Tables.

The respective values for these components vary with crops, soils, regions and seasons, so using region or plot specific data is most advised when available. Regional or global averages always hold a specific margin of error in estimation.

5. *Water Resources*

Water resources are defined by sources u and applications or uses v. Sources include groundwater, surface water, sea water, and grey water; while applications can be domestic, agricultural or industrial. This allows us to control water transfer from certain sources to specific uses, and track how the model chooses to allocate the available water given the different demands. Water treatment processes are also taken into account by an index w in order to transform a water source into its destination use.

6. *Energy Resources*

The energy component in the model is accounted for at three levels: the raw source e, the processing technology f, and the energy carrier g. This classification was necessary as each resource (e, f, g) demands a specific set of water, land, and energy footprints, and is characterized by different greenhouse gas emission rates (thus corresponding N and C footprints) which are all necessary for the formulation of the model results.

7. Climate, Soil, and Crop Characteristics

Climate, denoted by r, along with soil texture, denoted by s, determine crop water footprints, available green water, atmospheric deposition, biological nitrogen fixation, and crop yields. Crop yields were obtained from FAOSTAT as the average of 2010-2016 world yields. Potential yield is accounted for by adding 5% to the average yield as recommended by FAO. All water footprints for crops and food items were obtained from Mekonnen and Hoekstra (2011, 2012).

8. Land Resources

Land resources available are exploited for crop production, livestock grazing, and energy production. Pasture lands for livestock grazing are considered equal to those growing fodder crops and grasses.

9. Irrigation Techniques

Irrigation techniques q such as drip, sprinkler, and surface irrigation affect water losses and are characterized by their water use efficiency.

B. Model Framework

Figure 6 presents a flowchart illustrating the model relations and demonstrates the coupling of nitrogen into the three nexus pillars of water, energy and food. Shaded tabs represent the model’s primary decision variables. The model is multi-scale and follows the same spatial and temporal resolutions as those of Mortada et al. (2018).

Spatially, primary decision variables are solved at fine resolution (plot or farm) then aggregated to higher levels (district or group of adjacent districts) through auxiliary variables. The model is presented at a regional or national level, but with flexibility of dimension and region size. Temporally, the model also is multi-scale operating at fine resolution (weeks to months) for dynamic processes (like irrigation and fertilization) and aggregating to larger temporal scale (season to year) at other systems components, such as nutrient cycling, cropping seasons, livestock production, and national water, energy and food policies. However, a year-to-year balance was adopted to accommodate for the opposite ends of the timeframe.

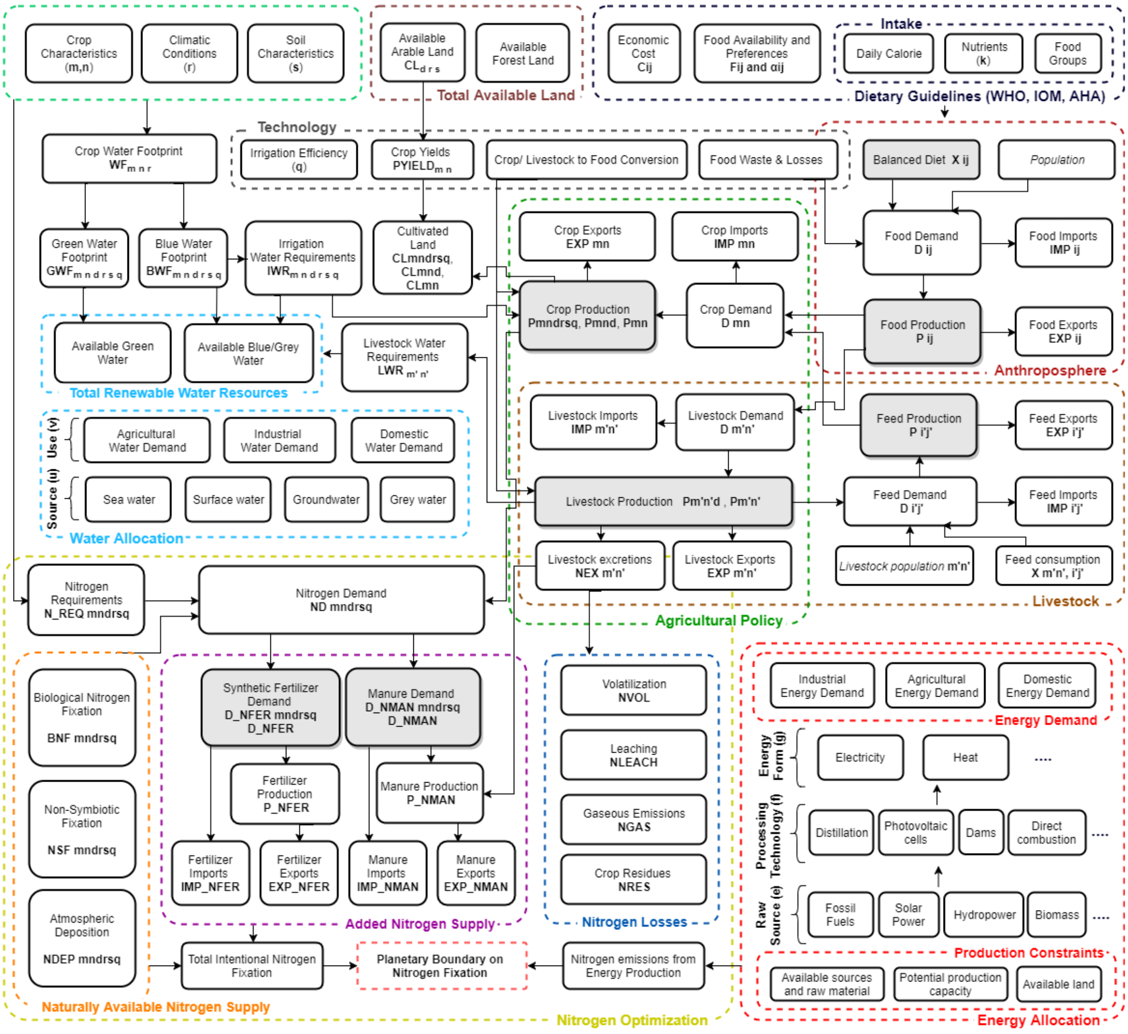


Figure 6: Model Flowchart

1. ***Decision Variables***

In addition to the original model variables of food and crops, we add the decision variables of livestock and feed, nitrogen application, as well as water and energy use. All decision variables are summarized in Table 21 of Appendix D: Model Decision Variables and Constraints.

a. Food consumption decision variables

At the individual scale, we introduce the individual food consumption variable. This remains the primary decision variable in the model. It is denoted by X_{ij} and represents the daily consumption per capita of food item (i, j) in g/capita/day. The total number of the decisions variables is $\sum_{i=1}^{I} J(i)$.

b. Food decision variables

D_{ij}, P_{ij}, IMP_{ij} and EXP_{ij} are respectively demand, production, import and export quantities of food items (i, j) per year in ton/year. Note that D_{ij} is an auxiliary decision variable directly related to X_{ij} by the food national demand constraint. Similarly, the total number of each of the four decisions variables is $\sum_{i=1}^{I} J(i)$.

c. Crop decision variables

D_{mn}, P_{mn}, IMP_{mn} and EXP_{mn} are respectively national domestic demand, production, import and export quantities of crop item (m, n) per year in ton/year. These variables are a direct consequence of food and feed demand, which is expressed in the food-crop and feed-crop relating constraints. The total number of each of the decisions variables *is* $\sum_{m=1}^{M} N(m)$.

Crop production is not only accounted for at the national level, but also at the smaller district level with P_{mnd}, and at the specific plot level P_{mndrsq}. P_{mndrsq} represents the production of crop (m, n) in district d, in climate r, in soil s, and under irrigation technique q. P_{mnd} and P_{mn} come as consequent auxiliary decision variables.

d. Feed decision variables

$D_{i'j'}$, $P_{i'j'}$, $IMP_{i'j'}$ and $EXP_{i'j'}$ are respectively demand, production, import and export quantities of feed items (i', j') per year in ton/year. These values are dependent on existing population, demand for livestock, and available land for feed crop production at the given district. The total number of each of the decisions variables is $\sum_{i'=1}^{I'} J'(i')$.

e. Livestock decision variables

$D_{m'n'}$, $P_{m'n'}$, $IMP_{m'n'}$ and $EXP_{m'n'}$ are respectively national domestic demand, production, import and export quantities of livestock (m', n') per year in animal/year. Similarly, the total number of each of the decisions variables is $\sum_{m'=1}^{M'} N'(m')$.

f. Fertilizer decision variables

D_N_{FER} , P_N_{FER}, IMP_N_{FER} and EXP_N_{FER} are respectively the nitrogen fertilizer demand, production, import and export quantities kgN/year. Nitrogen fertilizer demand is first determined at the scale of the crop, where $D\_N_{FER,mndrsq}$ in kgN/ha is the nitrogen fertilizer required for crop (m, n) in district d, climate r, with soil texture

s, and irrigation technique q. The total number of the decision variables is $DRSQ \sum_{m=1}^{M} N(m)$.

g. Manure decision variables

D_N_{MAN} , P_N_{MAN}, IMP_N_{MAN} and EXP_N_{MAN} are respectively the manure nitrogen demand, production, import and export quantities in district d in kgN/year. As fertilizers, manure demand is first determined at the scale of the crop, where $D\_N_{MAN,mndrsq}$ in kgN/ha is the manure required for crop (m,n) in district d, climate r, with soil texture s, and irrigation technique q. Manure production $P_{N_{MAN}}$ is limited by the existing livestock population. Similarly, the total number of the decision variables is $DRSQ \sum_{m=1}^{M} N(m)$.

h. Water resources decision variables

$P_{u,v,w}$ is defined as production of water source u, for use or quality v, using treatment technology w. D_v, P_u are respectively, water demand for use v and water production from source u, all in m^3/year.

i. Energy resources decision variables

D_e, P_e, IMP_e, EXP_e are respectively demand, production, import and export of energy source e.

D_g, P_g, IMP_g, EXP_g are respectively demand, production, import and export of energy carrier g.

P_{efg} is the production of energy carrier g, from source e, using processing technology f.

2. *Objective Functions*

a. Maximizing nitrogen use efficiency

The main aim of the nitrogen problem is maximizing nitrogen use efficiency, as it ensures optimal usage of nitrogen sources to meet production demands.

$$OF(1) = Max\ (NUE) \tag{1}$$

This will favour the use of crops with low nitrogen requirements and high removal rates. It will discourage the production of animal products as they are characterized by being very nitrogen inefficient.

NUE over the whole system is calculated as follows, with nitrogen inputs and outputs of both crops and animals summed over all districts considered.

$$NUE \ = \frac{N\ outputs}{N\ inputs} \tag{2}$$

$$N\ outputs = N\ outputs, crops \ + \ N\ outputs, animals \tag{3}$$

For crops, inputs are the different naturally available and added sources of nitrogen, while outputs are content of nitrogen in harvested crops:

$$N\ outputs, crops \ = \sum_{m=1}^{M} \sum_{n=1}^{N(m)} \sum_{d=1}^{D} \sum_{r=1}^{R} \sum_{s=1}^{S} \sum_{q=1}^{Q} N\ outputs_{\ mndrsq} \qquad \forall\ m, n, d, r, s, q \tag{4}$$

$$N\ inputs, crops \ = \sum_{m=1}^{M} \sum_{n=1}^{N(m)} \sum_{d=1}^{D} \sum_{r=1}^{R} \sum_{s=1}^{S} \sum_{q=1}^{Q} N\ inputs_{\ mndrsq} \qquad \forall\ m, n, d, r, s, q \tag{5}$$

$$N\ inputs_{mndrsq} = D\_N_{FER,mndrsq} + D\_N_{MAN,mndrsq} + NDEP_{mndrsq} + BNF_{mndrsq} + NSF_{mndrsq} \quad \forall\, m, n, d, r, s, q \tag{6}$$

$$N\ outputs_{mndrsq} = P_{mndrsq} \times N\ content_{mn} \times 1000 \quad \forall\, m, n, d, r, s, q \tag{7}$$

Where $N\ content_{mn}$ is nitrogen content in crop (m, n) in %.

For animal inputs and outputs, only dairy and meat food groups are considered. Nitrogen inputs are livestock intake of nitrogen through feed, and nitrogen outputs are content of nitrogen in animal-based food items.

$$N\ outputs, animals = \sum_{i=1}^{I} \sum_{j=1}^{J(i)} \left(P_{ij} \times N\ content_{ij} \times 1000\right) \quad \forall\, i, j\ \epsilon\ meat, dairy \tag{8}$$

$$N\ inputs, animals = \sum_{m'=1}^{M'} \sum_{n'=1}^{N'(i')} N\ inputs, animals_{m'n'} \quad \forall\, m', n' \tag{9}$$

$$N\ inputs, animals_{m'n'} = \sum_{i'=1}^{I'} \sum_{j'=1}^{J'(i')} \left(X_{i'j',m'n'} \times N\ content_{i'j'} \times 1000 \times Livestock\ population_{m'n'}\right) \quad \forall\, i', j', m', n' \tag{10}$$

Where:

- $N\ content_{ij}$ and $N\ content_{i'j'}$ are respectively nitrogen content in food (i, j) and feed (i', j') in %.

- $N\ outputs,\ N\ outputs, crops,\ N\ outputs, animals,\ N\ outputs, animals$ are in kgN/yr.

- $N\ inputs_{mndrsq}$, $Noutputs_{mndrsq}$ are in kgN/ha.

- $N\ inputs, animals_{m'n'}$ are in kgN/animal.

b. Minimizing nitrogen fixation

While NUE is an excellent indicator of nitrogen use, it does not give any idea on the magnitude of nitrogen applied, and consequently, lost to the environment. Even with high NUE values, the quantities of nitrogen lost to a specific ecosystem could still be detrimental, as they result from excessive nitrogen input originally. This nitrogen input is also important to us since it represents the planetary boundary concept on nitrogen, and the national status of nitrogen use.

$$OF(2) = Min\ (Total\ per\ capita\ nitrogen\ fixation) \tag{11}$$

where:

$$Total\ per\ capita\ nitrogen\ fixation = \frac{Total\ natural\ N\ fixation\ +\ Total\ added\ N}{population} \tag{12}$$

This problem will favour the production of crops and consumption of food items that have minimal nitrogen requirements, as well as the application of recycled nitrogen sources, namely animal manure, that results with lower losses over the introduction of external sources such as synthetic fertilizers.

3. Model Constraints

a. Food national demand and policy constraints

Food national demand in ton/year is calculated from individual food consumption X_{ij} in g/cap/day, accounting for food wastes and losses. Food wastes represent the portion of food lost in the stages of crop harvesting, distribution, and processing. Food losses are the portion of food lost at the consumption stage, or in households. Data for food wastes and losses are obtained from Gustavsson et al. (2011).

$$D_{ij} = \frac{X_{ij} * population * 365.25}{10^6 * \left(1 - waste\ factor_{ij}\right)\left(1 - loss\ ratio_{ij}\right)} \qquad \forall\ i\ \&\ j \qquad (13)$$

Consequently, food national balance is conducted at the end of each inventory year considering no stock changes:

$$P_{ij} + IMP_{ij} - EXP_{ij} = D_{ij} \qquad \forall\ i\ \&\ j \qquad (14)$$

b. Feed national demand and policy constraints

Similar to food demand, feed national demand is computed based on livestock groups population and their respective feed consumption rates.

$$D_{i'j'} = \sum_{m'=1}^{M'} \sum_{n'=1}^{N'} \left(X_{i'j',m'n'} * Livestock\ population_{m'n'}\right) \qquad \forall\ i'\ \&\ j' \qquad (15)$$

Where $X_{i'j',m'n'}$ is the consumption rate of feed item (i', j') by livestock (m', n') in ton/animal/year and $Livestock\ population_{m'n'}$ is the population of livestock type (m', n').

Accounting for feed import, export and production, the feed national balance is similarly conducted at the end of each inventory year considering no stock changes:

$$P_{i'j'} + IMP_{i'j'} - EXP_{i'j'} = D_{i'j'} \qquad \forall\ i'\ \&\ j' \qquad (16)$$

c. Modified crop-food and crop-feed relating constraints

Since our model takes livestock into account, the demand for fodder crops should account for that as well. This is why we add to the existing crop-food relating constraint, a term computing crop demand as feed for livestock.

$$(D_{mn}) = A \times (P_{ij}) + A' \times (P_{i'j'}) \qquad \forall\, m, n, i, j, i', j' \qquad (17)$$

Where:

$A = [a_{mn,ij}]$ is the crop-to-food conversion matrix first introduced by Mortada et al. (2018);

where $a_{mn,ij}$ is the amount of crop (m, n) required to produce a unit weight of food item (i, j).

Dimension of A is $\sum_{m=1}^{M} N(m) \times \sum_{i=1}^{I} J(i)$.

$A' = [a'_{mn,i'j'}]$ is the crop-to-feed conversion matrix, modified from matrix A;

where $a'_{mn,i'j'}$ is the amount of crop (m, n) required to produce a unit weight of feed item (i', j').

Dimension of A' is $\sum_{m=1}^{M} N(m) \times \sum_{i'=1}^{I'} J'(i')$.

The crop national balance at the end of each inventory year becomes the following:

$$P_{mn} + IMP_{mn} - EXP_{mn} = D_{mn} \qquad \forall\, m, n \qquad (18)$$

d. Crop production constraints

National crop production is an auxiliary decision variable calculated at two stages from production at the farming plot level to the district level. The following two constraints illustrate those two relations:

$$P_{mn} = \sum_{d=1}^{D} P_{mnd} \qquad \forall\, m \,\&\, n \tag{19}$$

$$P_{mnd} = \sum_{r=1}^{R} \sum_{s=1}^{S} \sum_{d=1}^{D} P_{mndrsq} \qquad \forall\, m, n \,\&\, d \tag{20}$$

e. <u>Nutritional constraints</u>

Food security is at the core of the model in Mortada et al. (2018), and equally so in ours as nitrogen plays a major contribution in food production. Food security is defined by WHO as a person’s “physical and economic access to sufficient, safe and nutritious food to meet their dietary needs and food preferences for a healthy and active life” (WHO, 1996). However, Mortada et al. (2018) translate food security to both an individual and a national scale. The former is defined by the recommended calorific intake and nutritional requirements set by WHO, IOM, and AHA; while the national scale is represented by the self-sufficiency status determined by national consumption, production, export and import of food.

A total of 16 macronutrients are considered for our model, denoted by k. NTR_{ijk} stands for amount in grams of nutrient k contained in 100 grams of food item (i, j). The total nutrient intake per capita per day is limited by their respective lower and upper bounds. In addition to the nutrient intake constraint, an additional constraint on food intake is set. It limits the daily per capita intake between a minimum and a maximum limit for every food group.

$$L_k \leq \sum_{i=1}^{I} \sum_{j=1}^{J(i)} \frac{NTR_{ijk}}{100} * \left(Edible\ portion\ of\ X_{ij}\right) \leq U_k \tag{21}$$

$$\forall\, k\, \epsilon\, \{1; 2; \ldots; K = 16\}$$

$$Min\ intake_{\,i} < \sum_{j=1}^{J(i)} X_{ij} < Max\ intake_{\,i} \qquad (22)$$

$$\forall\ i \in food\ groups\ covered\ by\ AHA$$

f. Livestock-food relating constraints

Similar to matrix A introduced by Mortada et al. (2018), we introduce a matrix $B' = [b'_{m'n',ij}]$ which relates meat and dairy food items to their livestock origin. Every element $b'_{m'n',ij}$ represents the number of animals needed of livestock type (m', n') to produce a unit weight of food item (i, j).

$$(D_{m'n'}) = B\ \times (P_{ij}) \qquad \forall\ m', n', i\ \&\ j \qquad (23)$$

Where:

$B = [b_{m'n',ij}]$

Dimension of B is $\sum_{m'=1}^{M'} N'^{(m')} \times \sum_{i=1}^{I} J(i)$

The livestock national balance at the end of each inventory year becomes the following:

$$P_{m'n'} + IMP_{m'n'} - EXP_{m'n'} = D_{m'n'} \qquad \forall m', n' \qquad (24)$$

g. Livestock-manure relating constraints

From the available livestock population, we are able to compute the potential for local manure production from livestock excretions. First, we compute livestock excretions as the following:

$$N\_EX = \sum_{m'=1}^{M'} \sum_{n'=1}^{N'(m')} (Livestock\ excretion_{m'n'} \times\ Livestock\ population_{m'n} \qquad (25)$$

$$\forall\ m', n'$$

Manure produced is calculated as the manure excretions excluding the fractions lost in other processes. We follow IPCC calculations here and account for fractions of livestock excretions that remain on the grassland during grazing, fractions that are lost as gaseous emissions and volatilized ammonia, as well as the fraction burned as fuel (IPCC, 2006b). Values for Δ are present in Table 17 in Appendix B: Data Tables.

$$P\_N_{MAN} = N\_EX * (1 - \Delta) \tag{26}$$

h. Nitrogen-crop relating constraints

Nitrogen requirement, ND_{mndrsq} in kgN/ha for a crop (m, n) is the amount of nutrient nitrogen needed for the optimal growth of the crop, under which nitrogen becomes a limiting factor for this growth. The values for nitrogen demand were calculated per FAO's "Optimizing Nitrogen Use on the Farm" Technical Paper and are shown in Table 15 of Appendix B: Data Tables. Nitrogen could be supplied from either fertilizers or manure, therefore we present:

$$ND_{mndrsq} = N\_REQ_{mndrsq} - \left(NDEP_{mndrsq} + BNF_{mndrsq} + NSF_{mndrsq}\right) \quad \forall\, m, n, d, r, s, q \tag{27}$$

$$ND_{mndrsq} = D_{N_{FER,mndrsq}} + D_{N_{MAN,mndrsq}} \quad \forall\, m, n, d, r, s, q \tag{28}$$

i. Fertilizer and manure nitrogen national balance constraints

Both manure and fertilizer demand can be met from the production, import and export of each. We define national fertilizer and manure demand by equations (29) and (30) respectively below:

$$D\_N_{FER} = \sum_{m=1}^{M} \sum_{n=1}^{N(m)} \sum_{d=1}^{D} \sum_{r=1}^{R} \sum_{s=1}^{S} \sum_{q=1}^{Q} D\_N_{FER,mndrsq} \qquad \forall\, m,n,d,r,s,q \tag{29}$$

$$D\_N_{MAN} = \sum_{m=1}^{M} \sum_{n=1}^{N(m)} \sum_{d=1}^{D} \sum_{r=1}^{R} \sum_{s=1}^{S} \sum_{q=1}^{Q} D\_N_{MAN,mndrsq} \qquad \forall\, m,n,d,r,s,q \tag{30}$$

The national balance for fertilizer and manure nitrogen becomes:

$$P\_N_{FER} + IMP\_N_{FER} - EXP\_N_{FER} = D\_N_{FER} \tag{31}$$

$$P\_N_{MAN} + IMP\_N_{MAN} - EXP\_N_{MAN} = D\_N_{MAN} \tag{32}$$

j. Planetary boundary on nitrogen fixation

The planetary boundary on intentional nitrogen fixation is converted from a total fixation limit to a per capita basis, and it is currently set at a value of 8.9 kgN/cap/yr. This allows evaluating the boundary at any scale. Intentional nitrogen fixation refers to all nitrogen contributing to agricultural or industrial production, whether through a natural process or added nitrogen from fertilizers and manure.

$$\begin{aligned} &Total\ natural\ N\ fixation \\ &= \sum_{m=1}^{M} \sum_{n=1}^{N(m)} \sum_{d=1}^{D} \sum_{r=1}^{R} \sum_{s=1}^{S} \sum_{q=1}^{Q} \left(NDEP_{mndrsq} + BNF_{mndrsq} + NSF_{mndrsq}\right) \\ &\qquad \forall\, m,n,d,r,s,q \end{aligned} \tag{33}$$

$$Total\ added\ Nitrogen = D\_N_{FER} + D\_N_{MAN} \tag{34}$$

$$\begin{aligned} &\frac{Total\ natural\ N\ fixation + Total\ added\ N}{Population} \\ &\leq per\ capita\ N\ fixation\ planetary\ boundary \end{aligned} \tag{35}$$

k. Land resources constraints

Every defined district d is characterized by an available land for agriculture and energy production. Based on energy and food demands, and the objective function studied, the model allocates land used for either processes. Cultivated land is computed as a ratio between crop production and its corresponding potential yield as stated in Equation (36) below. Total cultivated land TCL is the summation of the cultivated land over all crops and districts (Equation (37)), and is constrained by the total available land accounting for land used for energy production (Equation (38)).

$$\frac{P_{mndrsq}}{PYIELD_{mn}} = CL_{mndrsq} \qquad \forall\, m, n, d, r, s \,\&\, q \tag{36}$$

$$\sum_{m=1}^{M}\sum_{n=1}^{N(m)}\sum_{d=1}^{D}\sum_{r=1}^{R}\sum_{s=1}^{S}\sum_{q=1}^{Q} CL_{mndrsq} = TCL \qquad \forall\, m, n, d, r, s \,\&\, q \tag{37}$$

$$TCL + \mathit{Land\ for\ energy\ production} \leq \mathit{Total\ available\ land} \tag{38}$$

l. Water resources constraints

Water withdrawal P_u is constrained by available resources (Equation (39)) and by demands D_v for agriculture, energy production, and households (Equation

(40)). No water imports and exports are allowed.

$$P_u \leq \mathit{Available\ water\ resources} \tag{39}$$

$$\sum_{u=1}^{U} P_u = \sum_{v=1}^{V} D_v \tag{40}$$

m. Energy constraints

Energy is characterized by raw sources, processing technologies, and final energy carriers. Energy demands that should be met are on the level of both raw sources and energy carriers.

$$P_e + IMP_e - EXP_e = D_e \qquad \forall\, e \qquad (41)$$

$$P_g + IMP_g - EXP_g = D_g \qquad \forall\, g \qquad (42)$$

Raw source demand D_e is computed by accounting for the conversion factors from production of the energy carriers via technology f when converting energy source e to final carrier g.

$$D_e = \sum_{f=1}^{F(e)} \sum_{g=1}^{G} \left(\frac{P_{efg}}{Conversion\ Factor_{efg}} \right) \qquad \forall\, e, f, g \qquad (43)$$

Where:

$$P_g = \sum_{e=1}^{E} \sum_{f=1}^{F(e)} P_{efg} \qquad \forall\, e, f, g \qquad (44)$$

The demand for the final energy carrier D_g is calculated by accounting for energy needed for crop, livestock, and food production, in addition to energy needed for water withdrawal and for domestic use.

$$D_g = \sum_{m=1}^{M} \sum_{n=1}^{N(m)} D_{g,mn} + \sum_{m'=1}^{M'} \sum_{n'=1}^{N'(m')} D_{g,m'n'} + \sum_{i=1}^{I} \sum_{j=1}^{J(i)} D_{g,ij} + D_{g,water} + D_{g,domestic} \qquad \forall\, i, j, m, n, m', n', g \qquad (45)$$

n. Non-negativity constraints

All decision variables are non-negative.

CHAPTER IV

VALIDATION WITH HYPOTHETICAL CASE STUDY

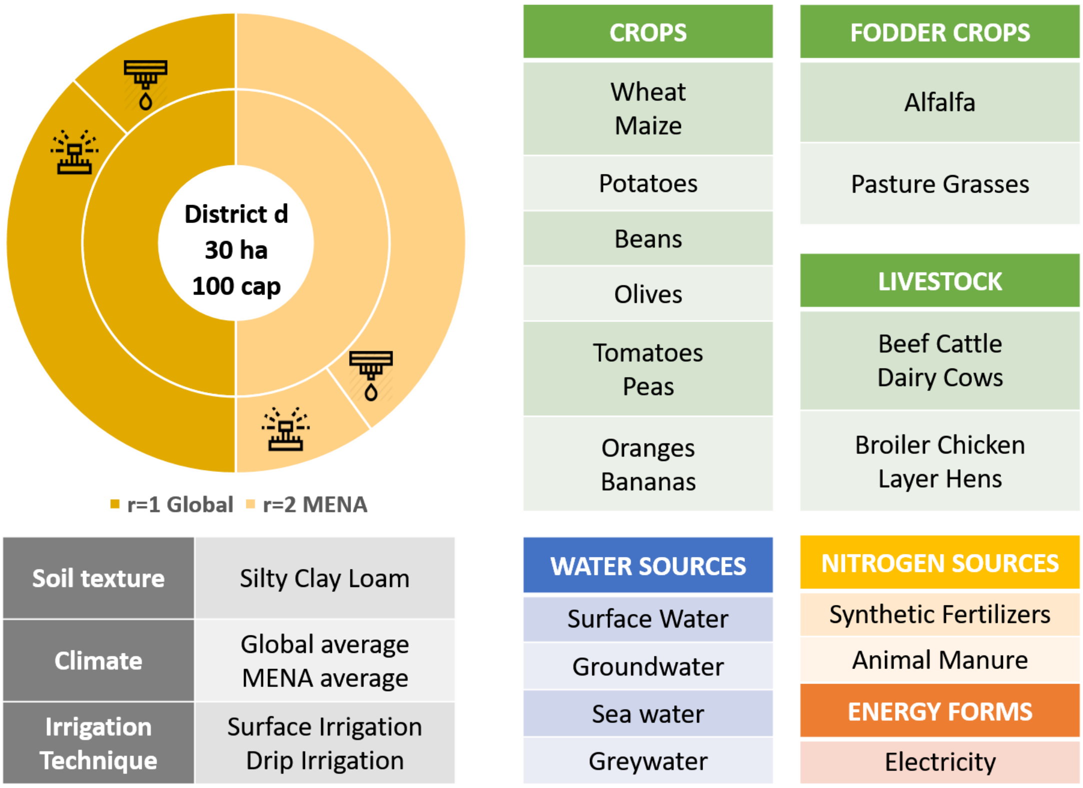
A. Description of the Case Study

To validate our model and test the proposed objective functions, we present a generic hypothetical case study. We consider one district d, consisting of two climates $(r = 1; r = 2)$ which determine the water footprints of the specified crops, with one soil texture s and two irrigation techniques ($q = 1;\ q = 2$). Climate 1 represents a global average, and climate 2 represents the MENA region climate. The soil is silty clay loam across the whole district, and irrigation techniques considered are sprinkler and drip irrigation characterized by different water efficiencies.

As for crops, we take 9 crops into account, in addition to two fodder crops. Two basic livestock groups, Cattle and Poultry, are added to evaluate the effect of animal products on the model results. For simplicity, three nutrients are accounted for: Water, Proteins, and Calories. Crops are chosen on a basis that they are fit to make up a fair diet, taking into account variations in their nutrient contents, and more importantly, their land, water, nitrogen, and energy footprints. We end up with 11 food items including drinking water.

When it comes to nitrogen, the nitrogen requirements for each crop were calculated and verified with data from the literature and common farmer practices. Yields, nitrogen requirements, and energy footprints of crops, livestock, food and feed items were considered similar across the two climates, equal to the global average (Climate 1). Only crop water footprints were calculated for each climate separately. Nitrogen requirements were set against water, energy and land (yield) footprints of the crops understudy in order to better understand the results of the model runs under each objective function. All data are summarized in Appendix C: Water, Energy, Land, Nitrogen Footprints.

For simplicity, limited but basic nutrients, energy forms, soil textures and irrigation techniques were considered. Those choices were taken on the basis of those components relative effect on the overall results of the case study, knowing that nitrogen is our main concern in this specific thesis. However, all adopted data was compared with literature values and global averages to ensure the case study provides a valid representation and is reliable to test and draw conclusions from. Appendix A: Case Study Data compiles the case study data for all the model components, and Figure 7 below summarizes the complete case study.



CROPS
Wheat Maize
Potatoes
Beans
Olives
Tomatoes Peas
Oranges Bananas

FODDER CROPS
Alfalfa
Pasture Grasses

LIVESTOCK
Beef Cattle Dairy Cows
Broiler Chicken Layer Hens

Soil texture	Silty Clay Loam
Climate	Global average MENA average
Irrigation Technique	Surface Irrigation Drip Irrigation

WATER SOURCES
Surface Water
Groundwater
Sea water
Greywater

NITROGEN SOURCES
Synthetic Fertilizers
Animal Manure

ENERGY FORMS
Electricity

Figure 7: Case study description

In summary, the developed case study compiles 214 decision variables and 228 constraints, knowing that not all original model constraints were taken into account. Objective functions OF (1) and OF (2) are assessed to evaluate the food security and nitrogen status of the model. The obtained model is non-linear non-convex, and Excel Premium Solver platform was used to perform the runs.

B. Adopted Approach

To go about testing our model, we develop five scenarios to evaluate our case study under the two objective functions presented. Those scenarios were developed in order to answer four specific research questions based on the broader questions mentioned early on in this thesis. The first “Baseline Scenario: Abundant Resources” was an obvious starting point not only as a control scenario for results comparison, but also as a scenario that allows us to compare the two objective functions: Maximizing NUE vs. Minimizing Nitrogen Fixation. This scenario illustrates the difference of targeting a low nitrogen input versus a high nitrogen use efficiency policy, answering research question (1). Research question (2) was branched into two more specific questions: the first is sensitivity of NUE and nitrogen fixation to limited water and land resources, evaluated through “Scenario 1: Limited Water Availability” and “Scenario 2: Limited Land Availability” ; the second is sensitivity of food security to variation in NUE and nitrogen fixation, evaluated through “Scenario 3: Decreasing per capita N fixation limit”. In Scenario 3, we limit the allowable application values of nitrogen, and observe how food security is ensured in response to the limited nitrogen fixation through maximizing NUE. In Scenario 4, we evaluate food security at the national level by relaxing self-sufficiency and assessing how far we are from the nitrogen fixation planetary boundary of 9 kgN/cap/yr. It is a simple attempt at estimating our ability to sustain self-sufficiency under planetary boundary policies.

All scenarios with their corresponding variables and studied objective functions are presented in Table 2 below.

Table 2: Description of the different case study scenarios

Scenario / Variables	***Baseline Scenario: Unlimited Resources***	***Scenario 1: Limited Water***	***Scenario 2: Limited Land***	***Scenario 3: Limited N fixation***	***Scenario 4: Relaxed SSRij***
Available Water (m^3)	300,000	300,000 → 0	300,000	300,000	300,000
Available Cropland (ha)	30	30	30 → 0	30	30
Nitrogen Fixation Limit (kgN/cap/yr)	30	30	30	30 → 0	30
SSR_{ij} = Production/ Demand	≥ 1	≥ 1	≥ 1	≥ 1	1 → 0
Objective functions studied	OF (1): Max NUE OF (2): Min N fix.	OF (1): Max NUE OF (2): Min N fix.	OF (1): Max NUE OF (2): Min N fix.	OF (1): Max NUE	OF (2): Min N fix.

C. Results and Sensitivity Analysis

1. Baseline Scenario: Abundant Resources

We first asses the status of the case study under the objective functions without any resource limitations and trade policies. However, the nitrogen fixation limit is set to 30 kgN/cap/yr at all times which is the lower threshold for nitrogen sufficiency level (upper threshold for the “no-nitrogen-stress” status), as we generally aim to limit affluent nitrogen application (Liu et al., 2010).

Table 3: Definition of nitrogen stress levels, from Liu et al. (2010)

N input to cropland (kgN/cap/yr)	***Nitrogen stress level***
>30	Nitrogen sufficiency
15–30	No nitrogen stress
9–15	Nitrogen stress
<9	Nitrogen scarcity

Besides the need to ensure a food security status at a national level, in our case, SSR_{ij} must be limited to be greater than or equal to 1 in all conditions. In both objective functions OF (1) and OF (2), the model tends to limit nitrogen use. Allowing import of food items will automatically force the model to import all food items to decrease local N fixation, and we won’t obtain a true interpretation of nitrogen use for crop production needs. Therefore, in this scenario and the following ones, all crop and food item imports are not allowed.

With 30 hectares of cropland and 110000 m^3 of water available, and no limitation on energy and fertilizer or manure import, we obtained the results summarized in Figure 8 below. No limits on diet variations were applied, therefore, the model might give radical solutions to meet the objective function targets. The figures below show the food variables, nitrogen variables, and resource use variables of the two objective functions under the Baseline Scenario. This scenario gives us a general idea on possible crop choices for the two different OFs and their corresponding trends in nitrogen and resource use.

We first notice bananas to be highly nitrogen efficient in both OFs as it is a dominant choice. For OF (1), maximizing NUE, we expect to also see peas, maize and beans, as they have high nitrogen removal rates. For OF (2), minimizing N fixation, we will expect to also see beans and maize as crop choices, as they should have low nitrogen requirements and possibly high yields (Figure 8).

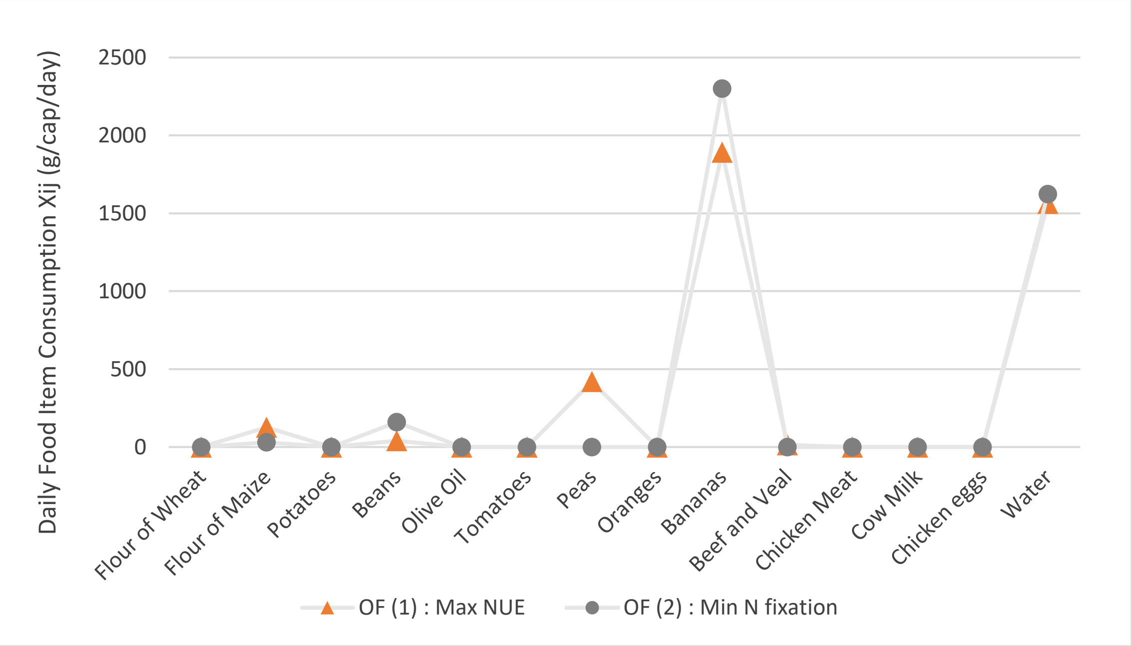


Figure 8: Food variables as per OF (1) and OF (2) under the Baseline Scenario

In Figure 9, we first notice that maximizing NUE meant a higher input of nitrogen in the proposed system. This may be explained by the fact that while the chosen crops might have high nitrogen removal rates, they also require high nitrogen application rates to grow. In fact, the nitrogen fixation limit of 30 kgN/cap/yr is a limiting constraint for OF (1) in this scenario. Another observation concerning nitrogen use is the distribution of manure and fertilizer application between the two OFs. OF (2) is more sensitive to the nitrogen source as it is a linear function, and therefore will always choose manure over fertilizer since part of it is recycled nitrogen from local animal excretions and it is associated with lower N losses.

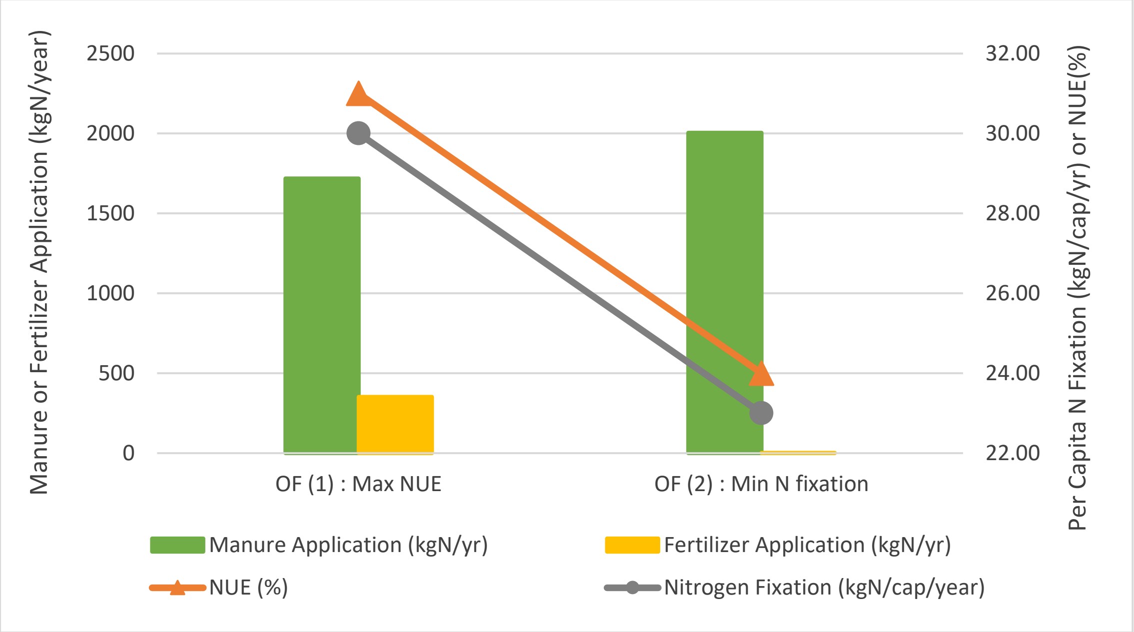


Figure 9: Nitrogen variables as per OF (1) and OF (2) under the Baseline Scenario

Finally, Figure 10 shows that OF (1) is more relaxed in resource use to maximize the total system NUE. This is evident in the usage of more land, water and energy. OF (2) on the other hand exploits 34% less land and 18% less water and energy. It is important to note that the available crop options are an important factor here. A wider and more diverse pool of crops with different yield, water, energy, and nitrogen characteristics might result with different conclusions.

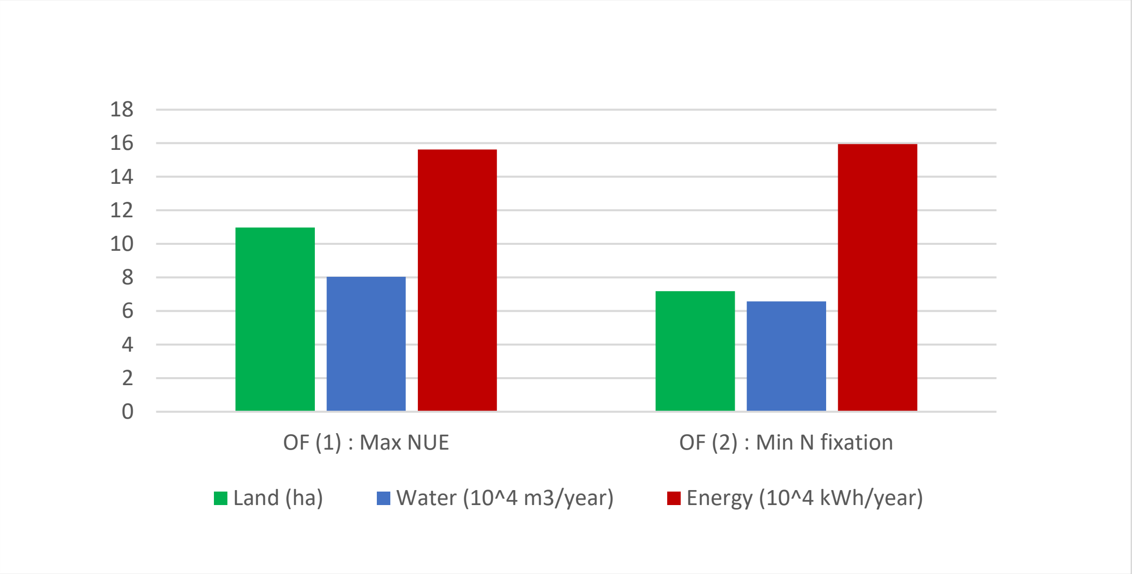


Figure 10: Resource variables as per OF (1) and OF (2) under the Baseline Scenario

2. *Scenario 1: Limited Water Availability*

Beyond the abundant resources scenario, we choose to limit water availability in this scenario to evaluate the sensitivity of NUE and N fixation to water crop and food processing requirements. We started with 50000 m^3/yr of available water and gradually decreased this value until no feasible solution was obtained, which was at around 11850 m^3/yr for both objective functions.

a. Sensitivity of OF (1) to water availability

Under this scenario, the model tries to obtain the combination of food items that achieves the highest NUE possible using limited water. Therefore, it should opt for both water and nitrogen efficient crops. In Figure 11, we can see that the favorable choice was bananas, along with flour of maize and beans. At 50,000m^3 of water available, a combination of oranges, potatoes and small amounts of bananas and flour was the most nitrogen efficient. At lower levels of water availability, 45000m^3 to 25000m^3, the dominant food item was bananas. However, somewhere between the 25000 and 20000m^3 marks, banana was no longer feasible water-wise, and the model switched to flour of maize to provide the nutritional demands while maintaining a relatively high NUE. Figure 13 supports that since it shows that water availability became a binding constraint at the 20000m^3 limit, but it also shows that achieving high NUE levels was also energy expensive.

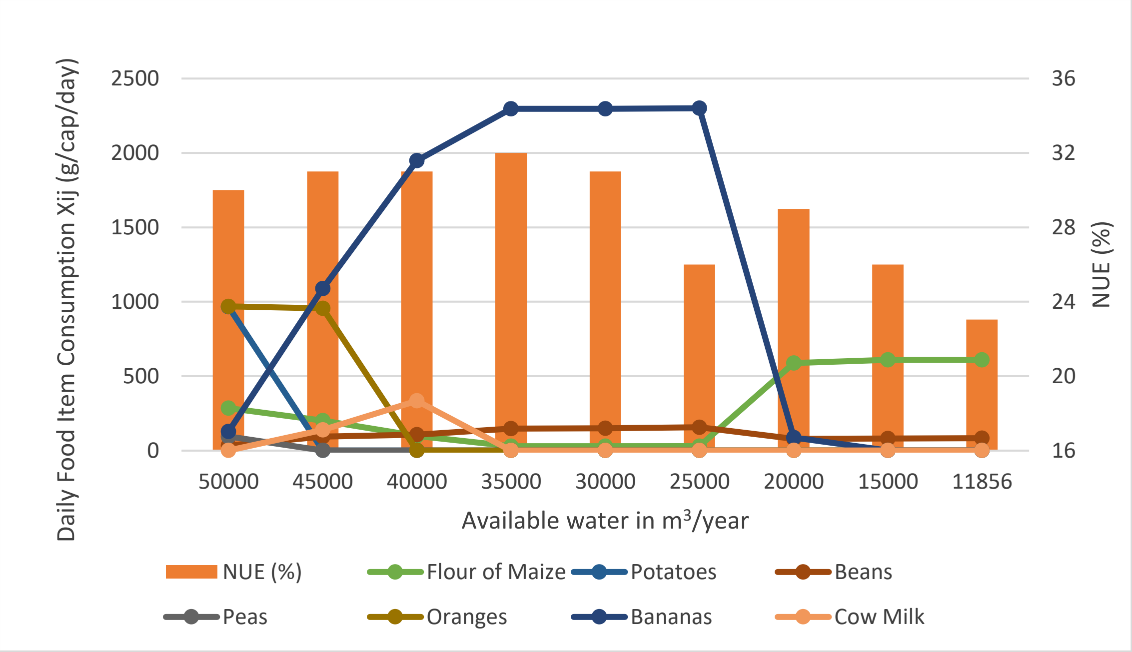


Figure 11: Food variables as per OF (1) under Scenario 1

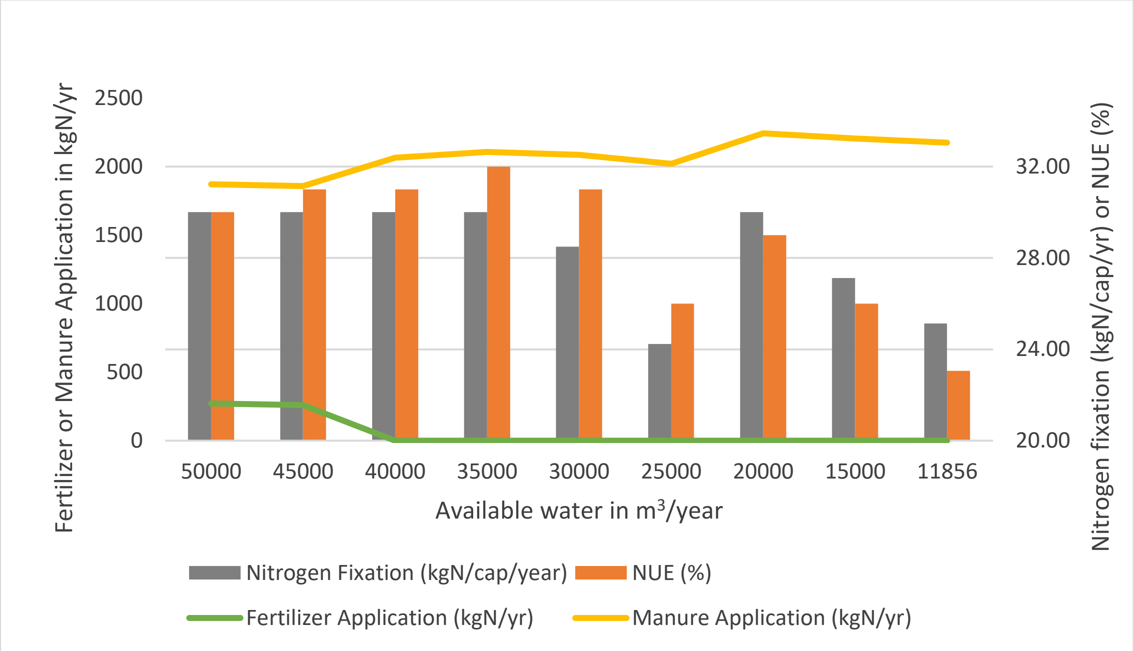


Figure 12: Nitrogen variables as per OF (1) under Scenario 1

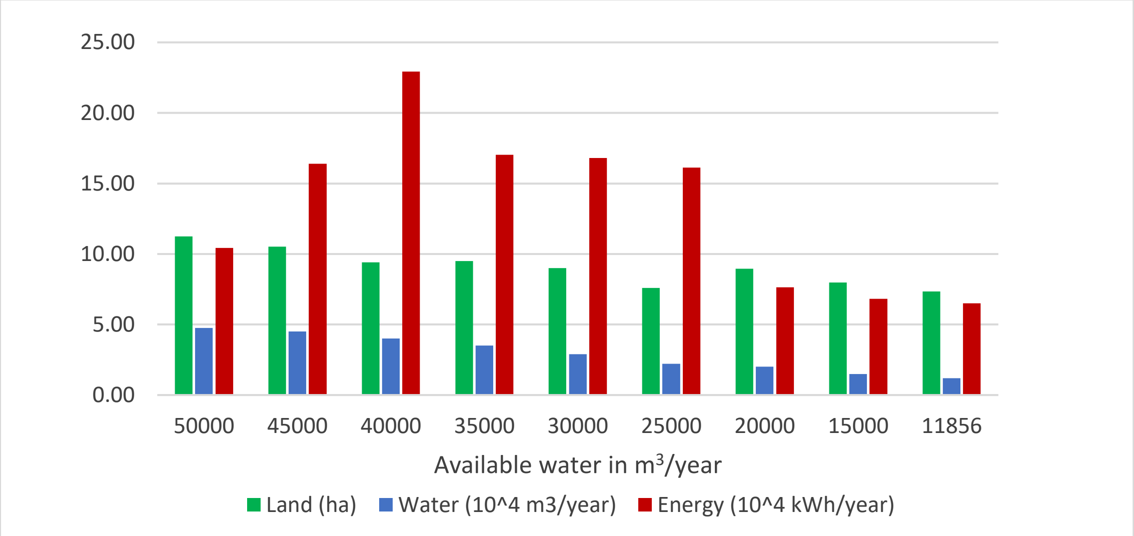


Figure 13: Resource variables as per OF (1) under Scenario 1

b. Sensitivity of OF (2) to water availability

Under limited water conditions, OF (2) is expected to suggest crops that require both low nitrogen and water inputs. In this scenario, we notice the same starting trend from 50000m^3 to 20000m^3 as that of Scenario 1, with bananas being the dominant choice. At water availability lower than 20000m^3, water became a limiting constraint for banana production, and the model switched to potatoes with a small amount of flour of maize since their combination was able to provide the nutritional demands with lower water requirements (Figure 14). Figure 16 even shows that water was not limiting for potato production at 15000m^3.

Figure 15 shows that compared to OF (1), OF (2) results with no use of synthetic fertilizers. NUE response to total N input is very predictable with NUE decreasing as N input increases.

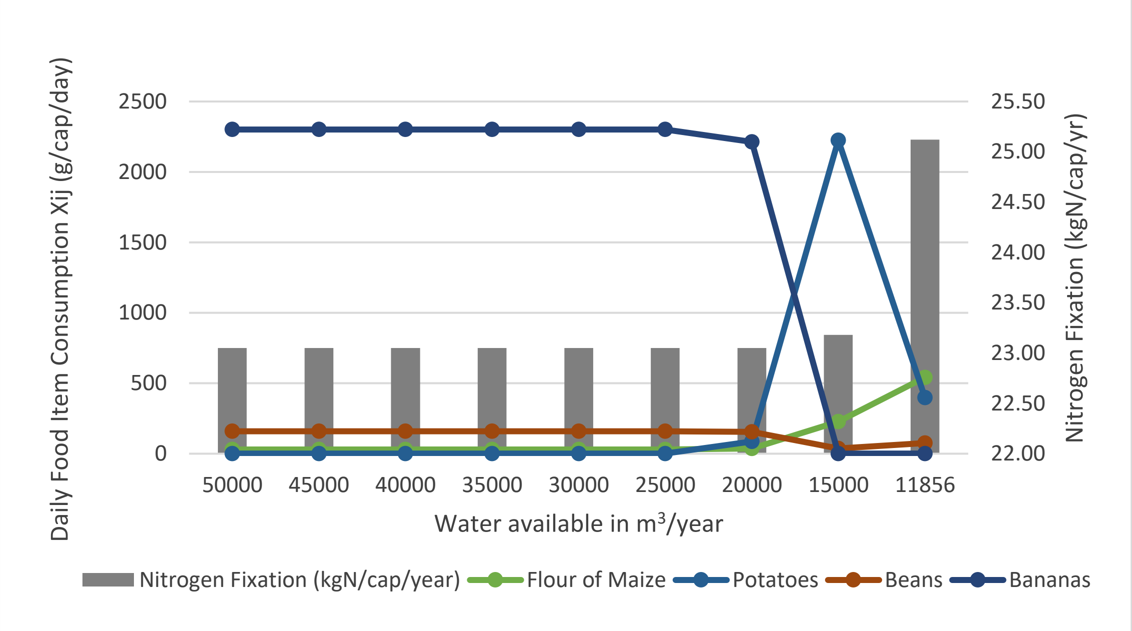


Figure 14: Food variables as per OF (2) under Scenario 1

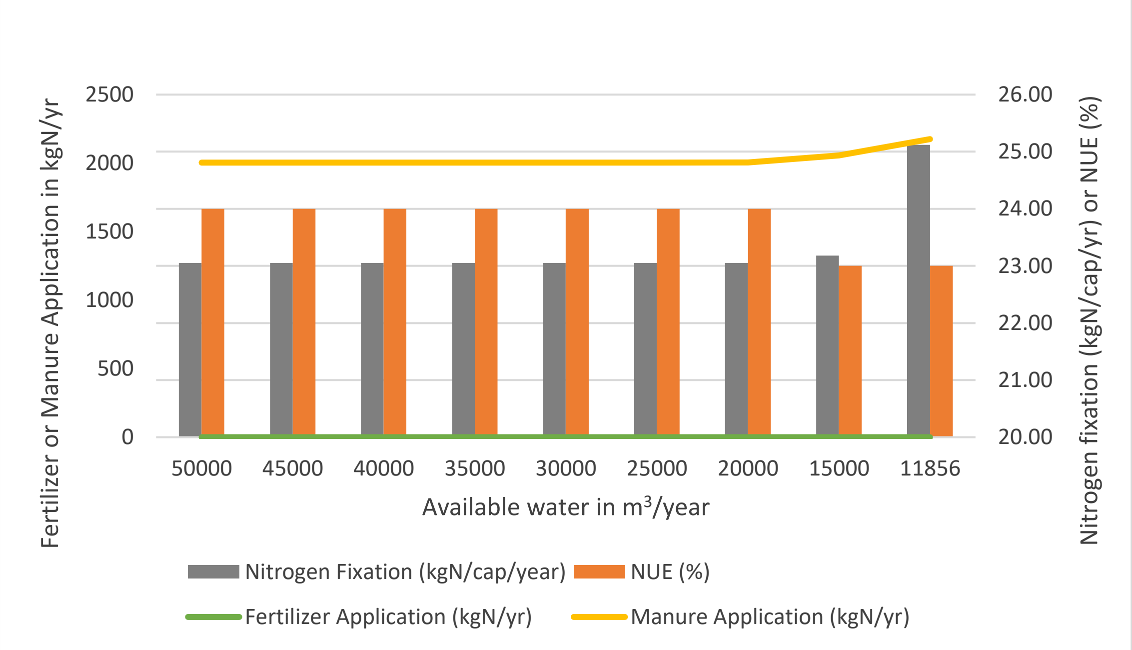


Figure 15: Nitrogen variables as per OF (2) under Scenario 1

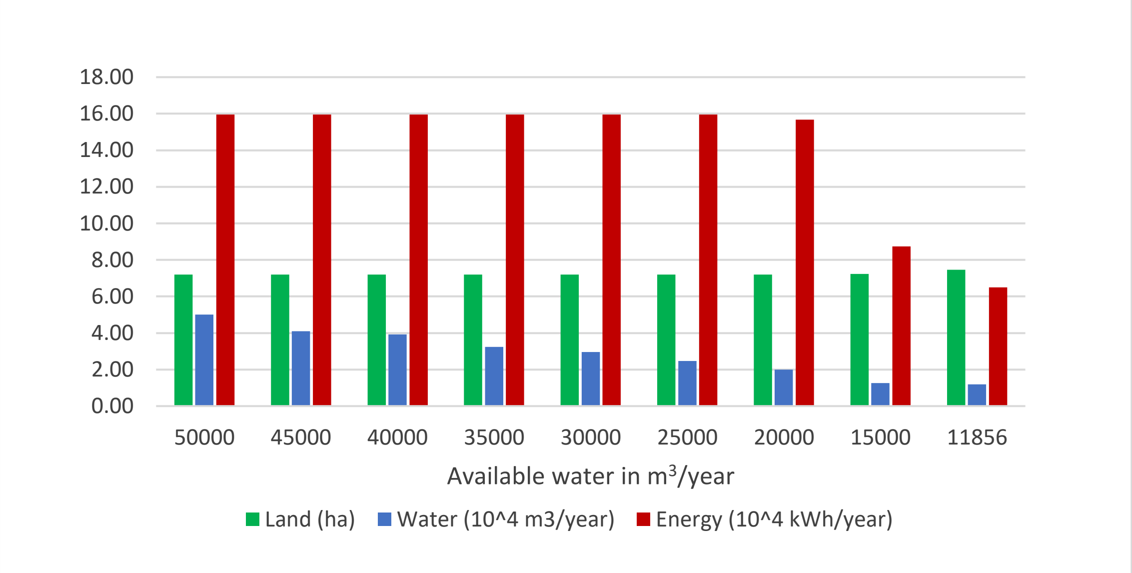


Figure 16: Resource variables as per OF (2) under Scenario 1

For both OFs applied under the limited water scenario, we conclude that no possible combination of crops can meet nutritional demands at water availability lower than 11850m^3. The highest NUE attainable at that limit was 23% producing maize and the lowest per capita N fixation was 25 kgN/cap/yr producing potatoes. The lowest land use value was observed under OF (1) with 7.33 ha exploited, while the minimum energy use was the same for both OFs with 650000 kWh consumed.

3. *Scenario 2: Limited Land Availability*

In this scenario, we choose to assess the sensitivity of NUE and N fixation to land availability. In OF (1), the model should opt for crops that have both high nitrogen removal rates and have high yields. In OF (2), the focus is on crops that require less nitrogen input in general. However, those two go hand in hand as a high yield crop already produces more with less amount of nitrogen applied compared to a lower yield crop with the same nitrogen requirements. This will be more evident in the results presented below.

a. Sensitivity of OF(1) to land availability

We started with 15 ha of cropland available to obtain the baseline scenario results and gradually decreased land availability. The first change was visible at 10.5 ha and we continued with a 1 ha decrease until no solution was found under the 7.5 ha limit. Food consumption, resource use and nitrogen use variations are presented in figures below respectively.

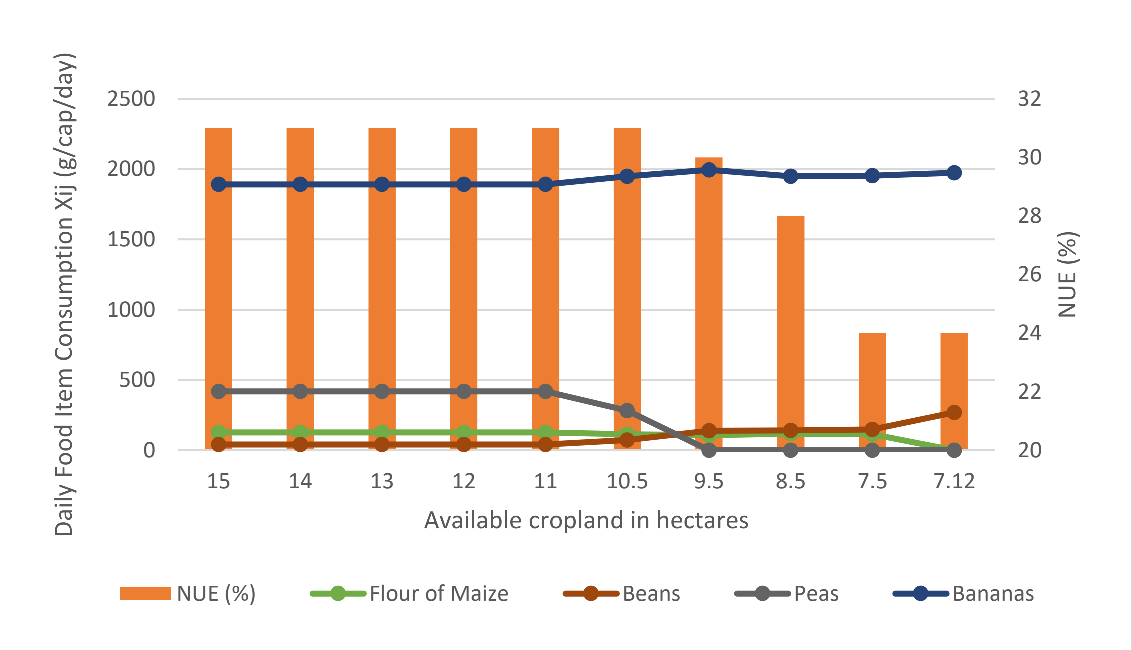


Figure 17: Food variables as per OF (1) under Scenario 2

Even under the limited land scenario, bananas, peas and beans remained a favoured choice. Bananas are a clear choice for their high yields, while peas and beans are highly nitrogen efficient (Figure 17).

Figure 18 shows that there's no clear correlation between the choice of synthetic fertilizers or manure to meet nitrogen requirements for crop production when it comes to optimizing nitrogen use efficiency. However, numbers show that total nitrogen applied increased from a range of 2000 kgN/yr to 2500 kgN/yr. This explains how, as available land was lowered, nitrogen use per capita increased and NUE decreased as a result.

Assessing the resource use variables under this scenario, we notice a very slight change in water and energy use, but we note that land availability was a limiting constraint all throughout (Figure 19). The final feasible solution was obtained at 7.12 ha, as the per capita nitrogen fixation hit the 30 kgN/cap/yr limit.

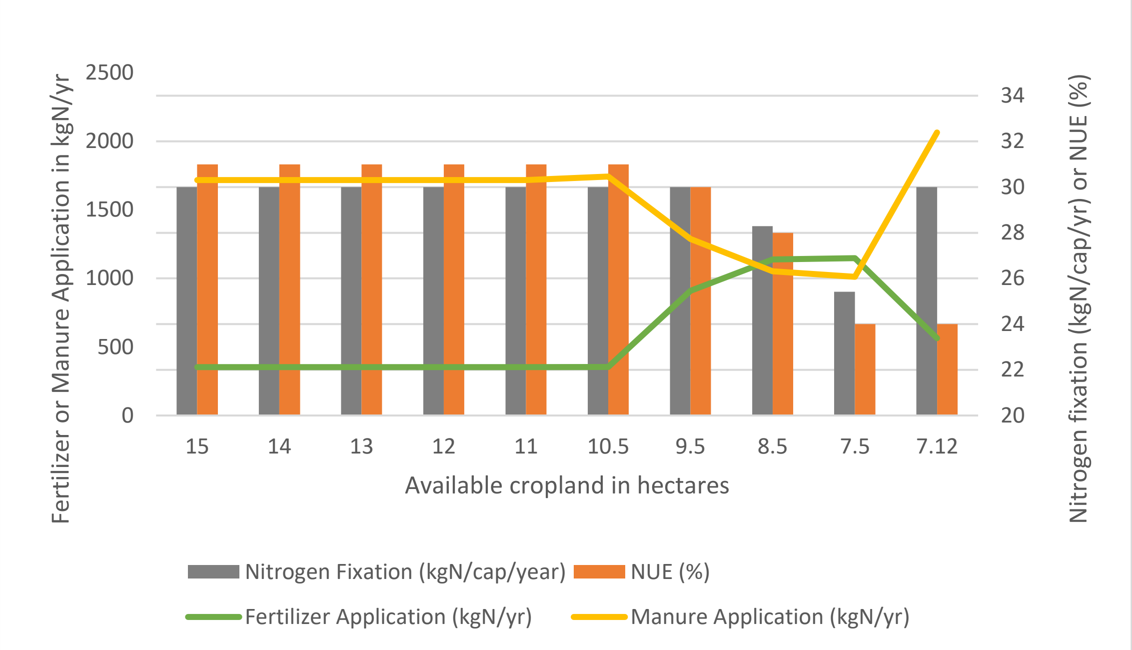


Figure 18: Nitrogen variables as per OF (1) under Scenario 2

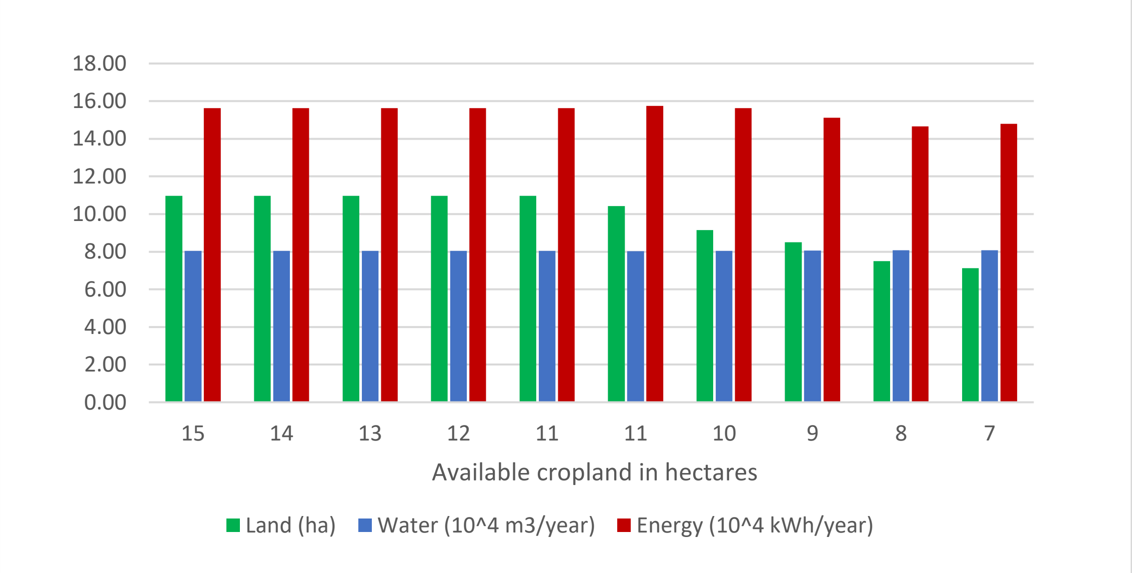


Figure 19: Resource use variables as per OF (1) under Scenario 2

b. Sensitivity of OF (2) to land availability

Similarly, we apply the limited land scenario to OF (2) to assess nitrogen fixation sensitivity to land availability. We should note how the baseline scenario of OF (2) already presented a low land exploitation of 7.19 ha. A value close to that of the minimum land used in OF (2) under Scenario 2. As expected, starting with 15 ha of land showed no effect on food choices or nitrogen fixation values until we approached the 7.19 ha mark. This supports the argument that the total nitrogen application is highly dependent on crop yields as it is on crop nutrient requirements. Minimizing nitrogen fixation led the model to directly opt for the high yield crops and therefore required much less land than maximizing nitrogen use efficiency did.

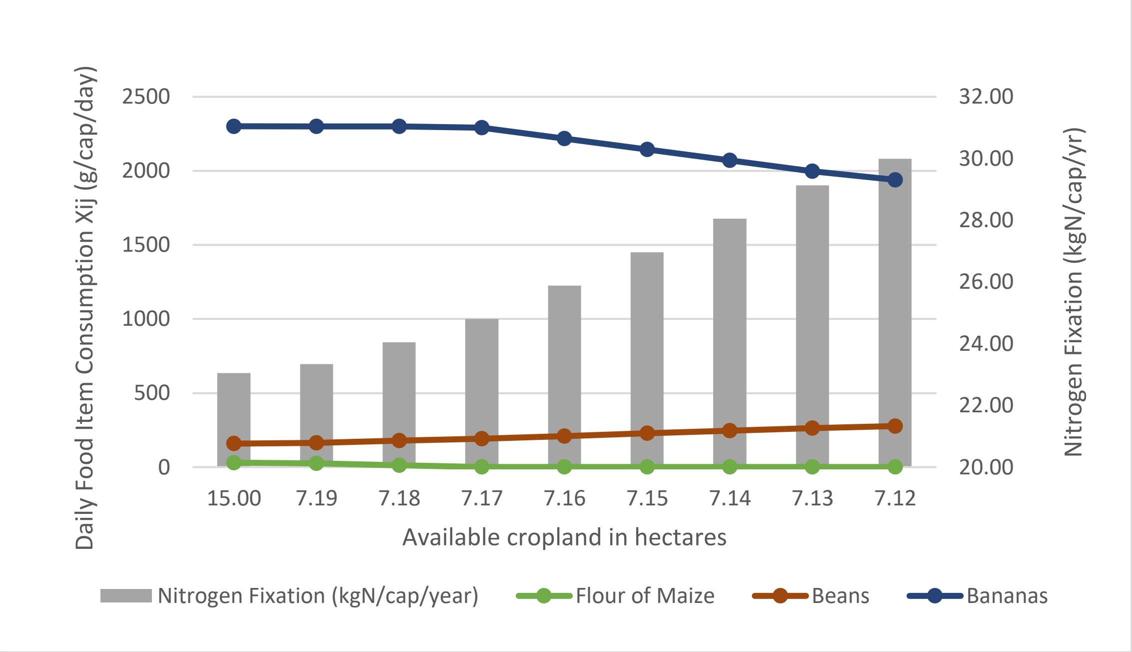


Figure 20: Food variables as per OF (2) under Scenario 2

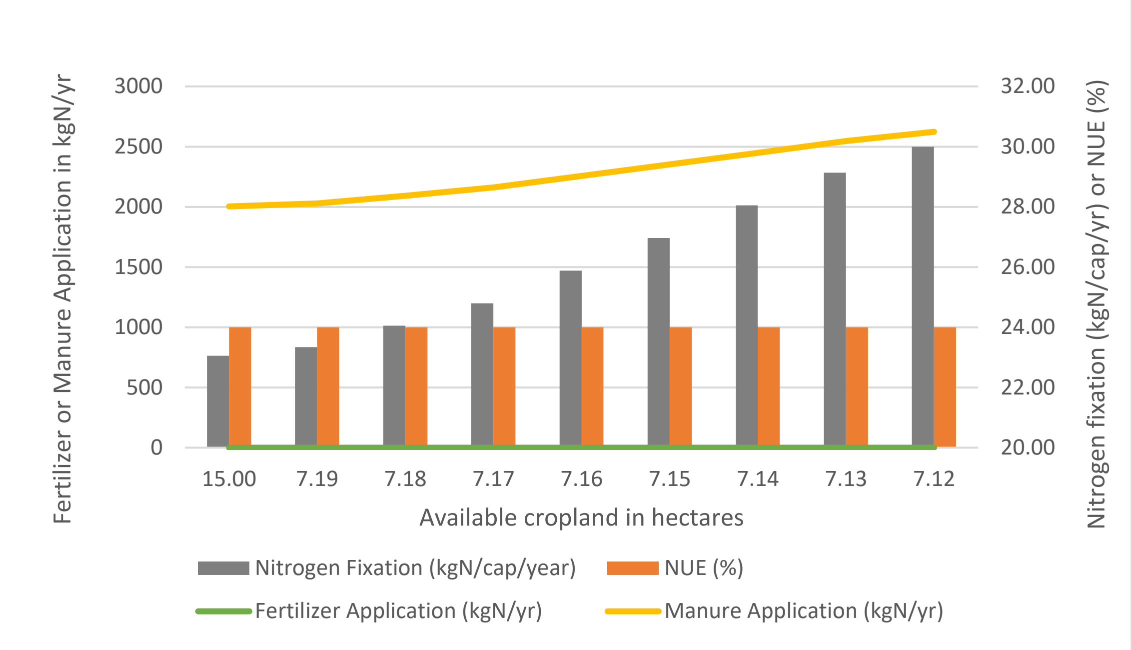


Figure 21: Nitrogen variables as per OF (2) under Scenario 2

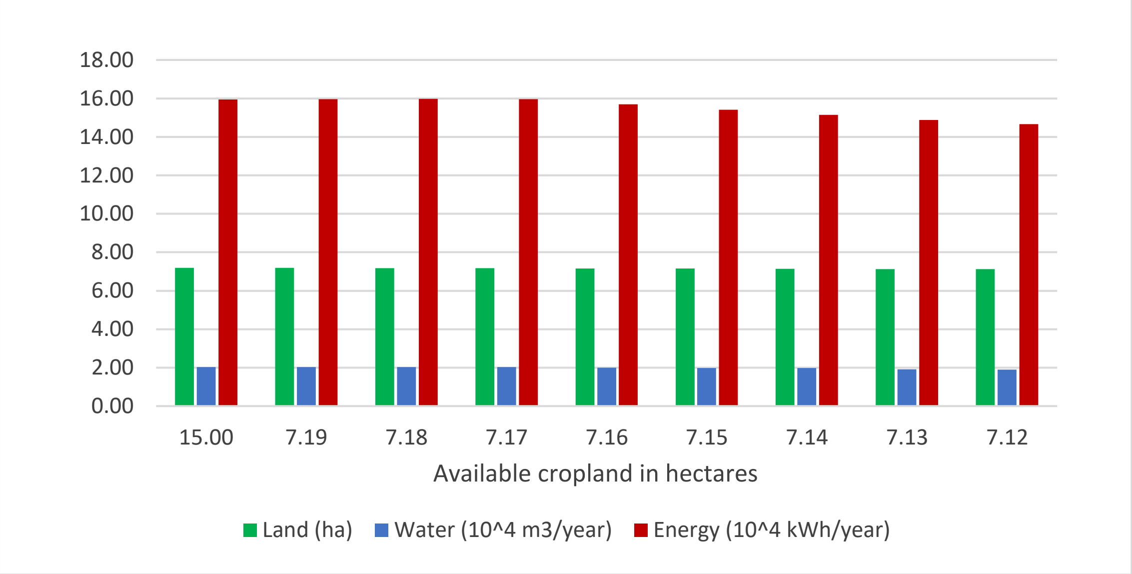


Figure 22: Resource use variables as per OF (1) under Scenario 2

Figure 20, Figure 21, and Figure 22 show the similar trends in food variables, water and energy use, and nitrogen fixation and efficiency between the two objective functions in response to land availability. Besides the difference in land use between OF (1) and OF (2), another apparent difference is the choice of nitrogen input. OF (2) once again favored the use of manure over synthetic fertilizers, and this was expected as the model doesn't relate the type of nitrogen used to crop yields. Therefore, OF (2) simply chooses manure because it is associated with lower losses, and results with lower required input.

A limited land scenario gave very similar crop and resource use trends as that of a limited water scenario. Both OF (1) and (2) gave no solution after the land available became lower than 7.12 ha. The highest NUE attainable was 24% and N fixation became a binding constraint reaching the 30 kgN/cap/yr limit as available land decreased. Minimum annual water and energy uses under this scenario were 19000m^3 and 146600 kWh respectively, observed under OF (2) at 7.12 ha of land available.

Both scenarios 1 and 2 of limited water and land availability show us that high NUE can come at an expense of high resource use; however, the effect of N fertilizers on crop yields needs to be incorporated in future research in order to obtain more significant and valid conclusions.

4. Scenario 3: Decreasing per capita N fixation limit

In Scenario 3, we're evaluating how high NUE can be maintained under limited nitrogen input conditions. Therefore, we apply OF (1) starting from the per capita N fixation limit of 30 kgN/cap/yr and gradually decrease the limit until we obtain no feasible solution. Figure 23 shows bananas, peas, beans and corn flour as the chosen food items, with no significant change from previous scenarios. The lowest N fixation limit that gave a feasible solution was 23.21 kgN/cap/yr, and at that level, NUE was at

24%. This scenario showed how with more restricted N fixation limits, we might no longer be able to meet our nutritional demands with a combination of nitrogen efficient crops, because they also need to have low nitrogen input requirements in addition to having high nitrogen removal rates. Therefore, there is a dire need to use recycled resources of nitrogen that come from crop residues, organic wastes, and animal manure, instead of constantly introducing new nitrogen to any cropland.

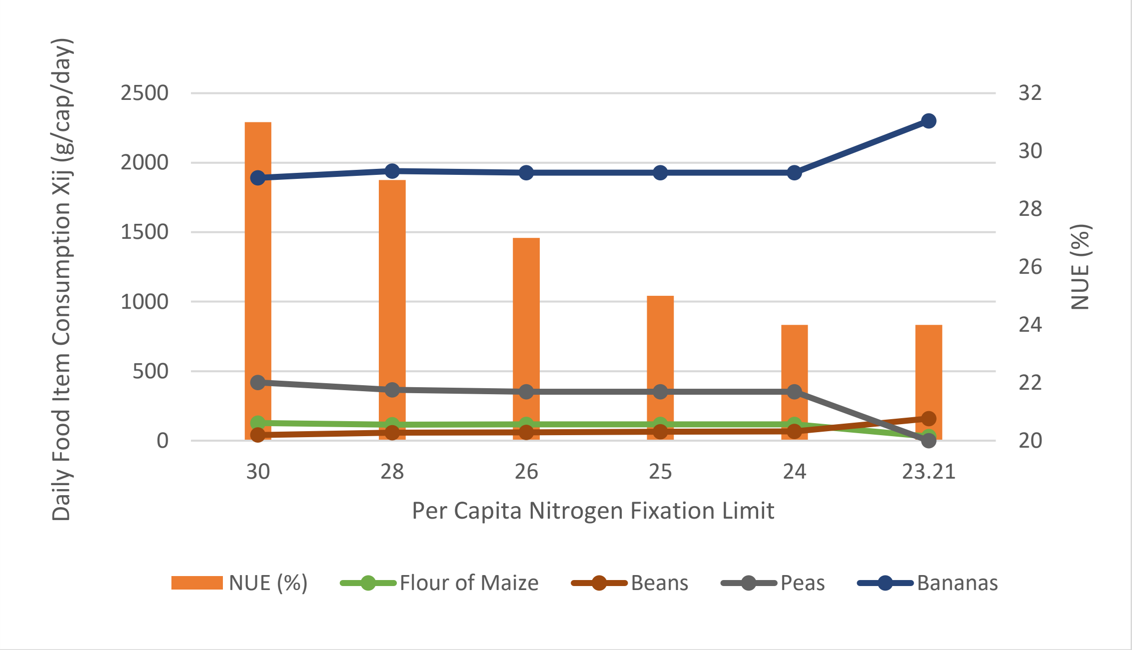


Figure 23: Food variables as per OF (1) under Scenario 3

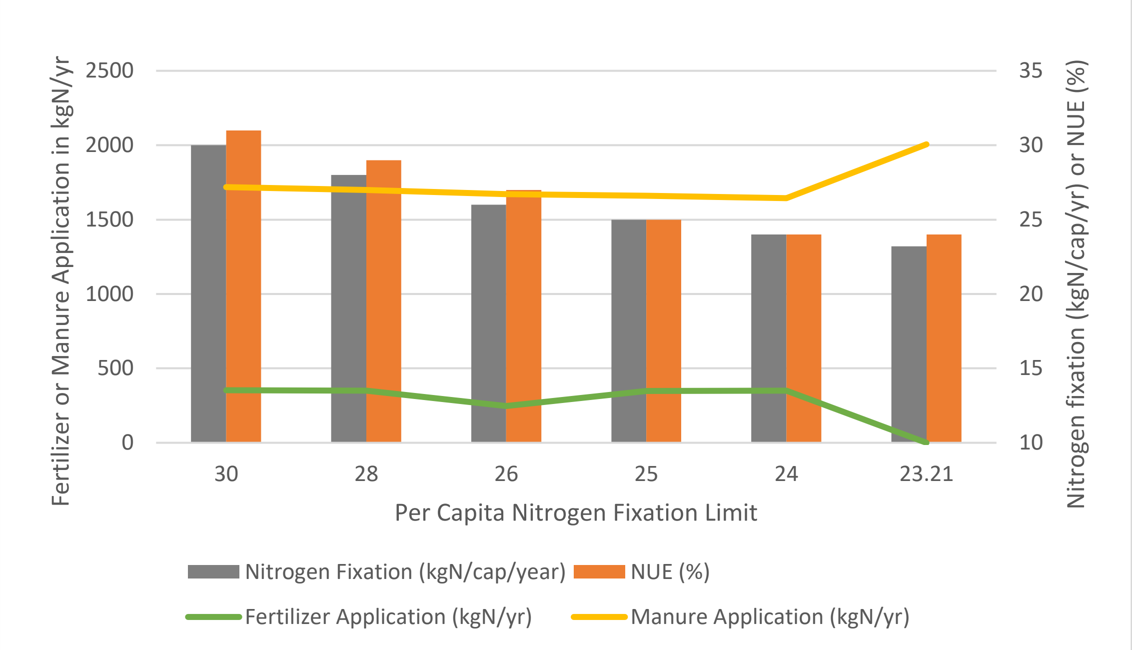


Figure 24: Nitrogen variables as per OF (1) under Scenario 3

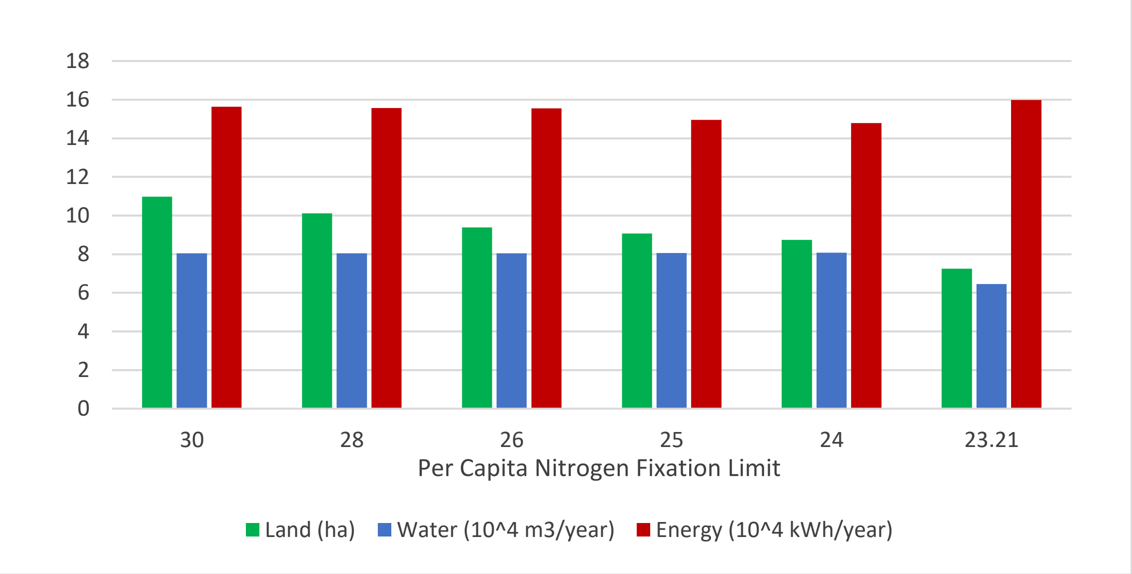


Figure 25: Resource use variables as per OF (1) under Scenario 3

5. *Relaxing Self-Sufficiency: How far are we from the nitrogen planetary boundary?*

The presented scenarios all resulted with a minimum N fixation rate of 23 kgN/cap/yr, which lies in the range of no nitrogen stress, and is very close to the global average of national nitrogen inputs. However, in order to stay within the planetary boundary of nitrogen, a level below 9 kgN/cap/yr should be achieved. In other words, agricultural systems should be managed as if under nitrogen scarcity conditions, aiming for high nitrogen use efficiencies, minimal losses, and optimal recycling rates, all while making sure not to deplete soils of its essential nitrogen. Using the baseline scenario results of OF (2), a simple calculation shows that annual nitrogen fixation needs to be lowered by 1400 kgN, or by 60%. On the other hand, the average added nitrogen applied to croplands is at 2000 kgN/yr (not accounting for natural nitrogen applied). Out of that nitrogen, 560 kgN/yr are retrieved in food, and 1440 kgN/yr are lost to the environment, 800 of which is accounted for as leaching, volatilization, and gaseous emissions. This leaves residual nitrogen at 640 kgN/yr, representing 45% of the 1400 kgN/yr excess nitrogen that needs to be compensated. At best, 50 % of this nitrogen could be recycled or avoided by adopting good agricultural practices and advanced technologies. In that case, the system is still more than 75% shy of achieving the planetary boundary limit while ensuring food security.

The above was tested out on OF (2) by relaxing the SSR_{ij} limit and allowing for food import until the 8.9 kgN/cap/yr mark was reached. The corresponding SSR_{ij} was 0.38. This means that, at this level of demand, in order to have a local fixation rate of 8.9 kgN/cap/yr, 62% of food demand cannot be locally produced, or 62% of nitrogen demand should be sought after in a sustainable manner rather than being introduced into the land at each season. This poses a risky dependency on external sources for food security, and this is a very simple example on how over exploiting our ecosystems to provide our food security, eventually leads to threatening those very ecosystems and our own food security once again.

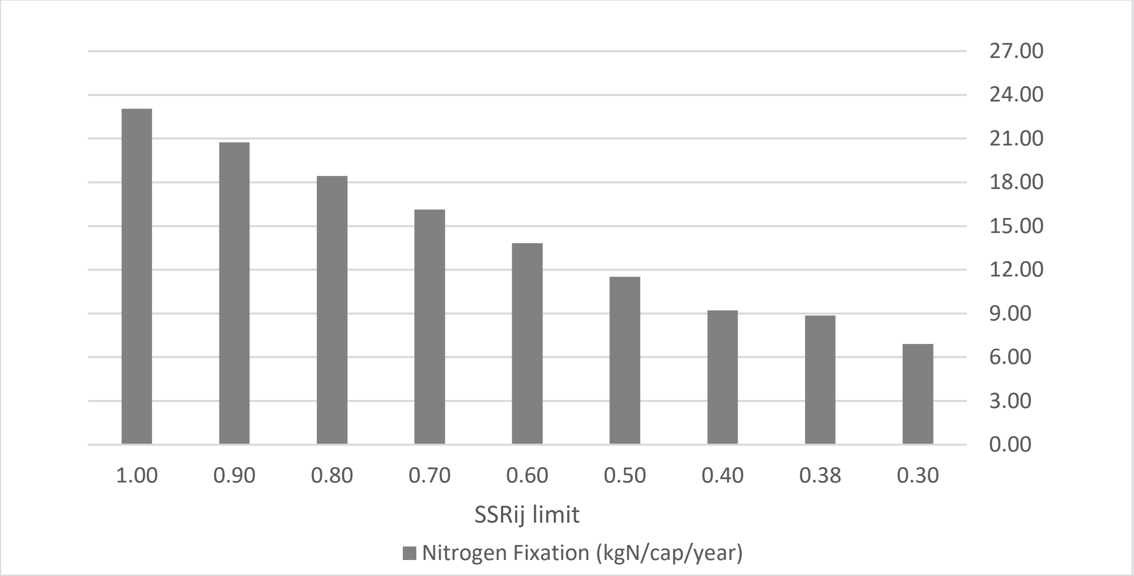


Figure 26: Response of nitrogen fixation values to decreasing the SSR_{ij} limit

CHAPTER V

CONCLUSIONS

In this thesis, we present an optimization model that helps decision makers take nitrogen-efficient choices under water, energy, and food security targets. The model is multi-scale, making it flexible to apply and tailor across farm, region, and nation-wide levels. A generic case study was developed to validate the model, and as simple as it may be, it illustrated the dependence of nitrogen variables on available natural resources, as well as dependence of food security on nitrogen. Maximizing the system nitrogen use efficiency always opted for crops with high N removal rates, but didn't account for their actual nitrogen input requirements, costing the system a very high per capita N fixation rate, and high amounts of N losses. On the other hand, minimizing nitrogen fixation always favoured organic and recycled nitrogen sources at all times as well as plant-based diets. For a 100-capita population, 15 ha of land, and 50000m^3 of water available, the highest NUE attainable was 32% and the lowest N fixation was 23 kgN/cap/yr. On the other hand, the model could not meet food security and environmental targets simultaneously when land was decreased below 7 ha and water below 12000m^3.

It is important to note that our model addresses the nitrogen problem from the supply side rather than the losses side. This means that it focuses on minimizing nitrogen input and maximizing nitrogen removal, given the available resources and technologies. On the losses side, we acknowledge that technologies and best management practices play a big role in reducing losses. Expanding the model to include additional factors such as effect of soil characteristics, climatic conditions, types of fertilizers used, and crop yield responses would add to the model’s effectiveness and accuracy. However, this requires quite an amount of data that is not easily available for such complex nexus problems.

Finally, a valuable improvement to the model would be adding the time factor, as it would allow to simulate real-life nexus applications taking the economic aspect into account, as well as incorporating cropping seasons and crop rotations which play a highly significant role in nitrogen management practices.

The main takeaways that this thesis was able to prove is that nitrogen fixation and nitrogen use efficiency should be studied in parallel when setting policy targets as a high NUE does not ensure a low nitrogen input and vice versa. Beyond nitrogen management itself, the WEF nexus illustrated significant dependency on nitrogen policies, and therefore those policies should be taken into consideration as a decision making factor when assessing the water, energy, or food security status.

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APPENDIX A: CASE STUDY DATA

Table 4: District, climate, soil and irrigation distribution

District	***Soil Texture***	***Climate***		***Irrigation Technique***		
d=1	s=1 Silty clay loam	r=1 Global	50%	q= 1	Sprinkler irrigation	26%
				q= 2	Drip irrigation	74%
		r=2 MENA	50%	q= 1	Sprinkler irrigation	81%
				q= 2	Drip irrigation	19%

Table 5: List of crops

Crop Group		***Crop Type***	
m=1	Cereals	n=1	Wheat
		n=2	Maize
m=2	Roots and tubers	n=1	Potatoes
m=3	Pulses (legumes)	n=1	Beans (dry)
m=4	Oil crops	n=1	Olives
m=5	Vegetables	n=1	Tomatoes
		n=2	Peas
m=6	Fruits	n=1	Oranges
		n=2	Bananas
m=7	Fodder	n=1	Alfalfa
		n=2	Grasses

Table 6: List of livestock

Livestock Group		***Livestock Type***	
m'=1	Cattle	n'=1	Beef Cattle
		n'=2	Dairy Cows
m'=2	Poultry	n'=1	Broilers
		n'=2	Laying hens

Table 7: List of food items

Food Group		***Food Item***	
i=1	Cereals	j=1	Flour of wheat
		j=2	Flour of maize
i=2	Roots and tubers	j=1	Potatoes
i=3	Pulses (legumes)	j=1	Beans (dry)
i=4	Vegetable oils	j=1	Olive oil, virgin
i=5	Vegetables	j=1	Tomatoes
		j=2	Peas
i=6	Fruits	j=1	Oranges
		j=2	Bananas
i=7	Meat	j=1	Beef and veal, Boneless
		j=2	Chicken meat
i=8	Dairy	j=1	Cow milk, whole, fresh
		j=2	Chicken eggs, with shell
i=9	Water	j=1	Water, tap, drinking

Table 8: List of feed types

Feed Group		***Feed Type***	
i'=1	Concentrates	j'=1	Wheat
		j'=2	Grain corn
i'=2	Roughages	j'=1	Grazing pasture
		j'=2	Dry hay
		j'=3	Silage

Table 9: Water sources and uses

Water Source	
u=1	Surface water
u=2	Groundwater
u=3	Sea water
u=4	Grey water

Water Use	
v=1	Agricultural
v=2	Industrial
v=3	Domestic

Table 10: Energy sources and carriers

Raw source	***Processing Technology***
e=1 Petroleum	f=1 Distillation
e=2 Natural Gas	f=1 Processing
e=3 Solar	f=1 Photovoltaics
e=4 Biomass	f=1 Maize (Direct combustion)
e=5 Hydropower	f=1 Medium-head dam
e=6 Wind	f=1 On shore

Energy Carrier	
g=1	Electricity

Table 11: Nutrients

Nutrient k		***lower bound***	***upper bound***	
k=1	Water	3200	-	g/cap/day
k=2	Energy	2500	2500	kcal/cap/day
k=3	Protein	62.5	93.75	g/cap/day

APPENDIX B: DATA TABLES

Table 12: Food items nutritional data

Food Group	*Food Item*	*Water g/100g*	*Energy kcal/100g*	*Protein g/100g*
i=1 Cereals	j=1 Flour of wheat	11.92	364.00	10.33
	j=2 Flour of maize	10.91	361.00	6.93
i=2 Roots and tubers	j=1 Potatoes	81.58	69.00	1.68
i=3 Pulses (legumes)	j=1 Beans (dry)	11.32	333.00	23.36
i=4 Vegetable oils	j=1 Olive oil, virgin	0.00	884.00	1.03
i=5 Vegetables	j=1 Tomatoes	94.52	18.00	0.88
	j=2 Peas	78.86	81.00	5.42
i=6 Fruits	j=1 Oranges	86.75	47.00	0.94
	j=2 Bananas	74.91	89.00	1.09
i=7 Meat	j=1 Beef and veal	61.94	254.00	17.17
	j=2 Chicken meat	75.46	119.00	21.39
i=8 Dairy	j=1 Cow milk	88.13	61.00	3.15
	j=2 Chicken eggs	87.57	52.00	10.90
i=9 Water	j=1 Water	99.90	0.00	0.00

Table 13: Food items characteristics

Food Group	*Food Item*	*Losses*	*Wastes*	*Edible portion*	*Priority*
i=1 Cereals	j=1 Flour of wheat	8%	15%	100%	1.00
	j=2 Flour of maize	8%	15%	100%	2.00
i=2 Roots and tubers	j=1 Potatoes	5%	15%	100%	2.00
i=3 Pulses (legumes)	j=1 Beans (dry)	5%	15%	100%	2.00
i=4 Vegetable oils	j=1 Olive oil, virgin	0%	15%	100%	2.00
i=5 Vegetables	j=1 Tomatoes	10%	15%	100%	2.00
	j=2 Peas	10%	15%	100%	2.00
i=6 Fruits	j=1 Oranges	10%	15%	100%	2.00
	j=2 Bananas	10%	15%	90%	2.00
i=7 Meat	j=1 Beef and veal	0%	15%	100%	1.00
	j=2 Chicken meat	0%	15%	100%	1.00
i=8 Dairy	j=1 Cow milk	4%	15%	100%	1.00
	j=2 Chicken eggs	10%	15%	100%	2.00
i=9 Water	j=1 Water	0%	15%	100%	1.00

Table 14: Natural nitrogen inputs to crops in kgN/ha

Crop Group	***Crop Type***	***Nitrogen Deposition ($NDEP_{mndrsq}$)***	***Biological N Fixation (BNF_{mndrsq})***	***Non-Symbiotic Fixation (NSF_{mndrsq})***
m=1 Cereals	n=1 Wheat	15.00	22.33	5.00
	n=2 Maize	15.00	14.52	5.00
m=2 Roots and tubers	n=1 Potatoes	15.00	0.00	5.00
m=3 Pulses (legumes)	n=1 Beans (dry)	15.00	240.00	25.00
m=4 Oil crops	n=1 Olives	15.00	12.29	5.00
m=5 Vegetables	n=1 Tomatoes	15.00	0.00	5.00
	n=2 Peas	15.00	44.04	5.00
m=6 Fruits	n=1 Oranges	15.00	0.00	5.00
	n=2 Bananas	15.00	0.00	5.00
m=7 Fodder	n=1 Alfalfa	15.00	390.00	5.00
	n=2 Grasses	15.00	29.45	5.00

Table 15: Crop nitrogen requirements calculations (given in kgN/ha)

Crop Group	***Crop Type***	***N required (N_REQ_{mndrsq})***	***N deficit***	***N to be added (ND_{mndrsq})***
m=1 Cereals	n=1 Wheat	81.60	60.46	120.92
	n=2 Maize	91.25	74.00	147.99
m=2 Roots and tubers	n=1 Potatoes	79.60	69.61	139.21
m=3 Pulses (legumes)	n=1 Beans (dry)	-	-	20.00
m=4 Oil crops	n=1 Olives	-	-	80.00
m=5 Vegetables	n=1 Tomatoes	76.06	66.06	132.13
	n=2 Peas	100.31	68.29	136.59
m=6 Fruits	n=1 Oranges	41.28	31.28	62.56
	n=2 Bananas	55.13	45.12	90.25
m=7 Fodder	n=1 Alfalfa	-	-	50.00
	n=2 Grasses	-	-	20.00

Sources for Tables 13, 14, 15: (Anglade et al., 2015; FAO, 2003; Godinot et al., 2014; Herridge et al., 2008; IFA, 1992; Ruiz et al., 2002)

Table 16: Nitrogen loss factors from nitrogen input

	Denitrification	***Volatilization***	***Leaching***
Nitrogen fertilizers	0.010	0.150	0.300
Manure used as fertilizer	0.006	0.100	0.300
Grazing animal dung and urine	0.010	0.150	0.300

Sources for Table 16: (Hofstra and Bouwman, 2005; IPCC, 2006a, 2006b)

Table 17: Nitrogen excretion factors from livestock

Livestock Group	***Livestock Type***	***Nitrogen Excretions (kgN/head/yr)***	***Fraction of excretions lost in manure management (Δ)***
m'=1 Cattle	n'=1 Beef Cattle	51.250	45%
	n'=2 Dairy Cows	73.125	22%
m'=2 Poultry	n'=1 Broilers	0.600	50%
	n'=2 Laying hens	0.600	50%

Sources for Table 17: (IPCC, 2006a, 2006b)

APPENDIX C: WATER, ENERGY, LAND, NITROGEN FOOTPRINTS

In tables 18, 19, and 20 below, color grading is used for footprint comparison. Darker shades represent higher footprint and thus higher environmental impact.

Table 18: Comparison of crop yields, water and energy footprints, and N fertilizer requirements

Crop Group	***Crop Type***	***Crop Yield ton/ha***	***Total Crop (Blue+ Green+ Grey) Water Footprint m^3.ton crop^{-1}***		***Crop energy requirement kWh. ton crop^{-1}***	***Crop N fertilizer requirement kgN/ha***
			r=1 Global	***r=2 MENA***		
m=1 Cereals	n=1 Wheat	3.22	1826	2045	1989	121
	n=2 Maize	5.36	1222	1037	1094	148
m=2 Roots and tubers	n=1 Potatoes	19.29	287	281	604	139
m=3 Pulses (legumes)	n=1 Beans(dry)	5.00	5053	3256	2142	20
m=4 Oil crops	n=1 Olives	1.90	3014	4069	2008	80
m=5 Vegetables	n=1 Tomatoes	35.18	214	191	806	132
	n=2 Peas	7.53	595	2028	666	137
m=6 Fruits	n=1 Oranges	17.87	560	625	536	63
	n=2 Bananas	20.58	790	691	1262	90
m=7 Fodder	n=1 Alfalfa	15.00	254	254	479	50
	n=2 Grasses	11.00	254	254	0.00	20

Table 19: Comparison of livestock water and energy footprints

Livestock Group	***Livestock Type***	***Total Water Footprint (Blue+ Green+ Grey) m^3. animal^{-1}***	***Animal Energy Requirement kWh. animal^{-1}***
m'=1 Cattle	n'=1 Beef Cattle	32.4	313
	n'=2 Dairy Cows	43	17196
m'=2 Poultry	n'=1 Broilers	0.03	0.62
	n'=2 Laying hens	0.20	15.14

Table 20: Comparison of food items water and energy footprints

Food Group	***Food Item***	***Total food (Blue+ Green+ Grey) Water Footprint m^3.ton food^{-1}***		***Crop Energy requirement kWh.ton food^{-1}***
		r=1 Global	***r=2 MENA***	
i=1 Cereals	j=1 Flour of wheat	22	22	562.51
	j=2 Flour of maize	31	31	562.51
i=2 Roots and tubers	j=1 Potatoes	0	0	0.00
i=3 Pulses (legumes)	j=1 Beans (dry)	0	0	0.00
i=4 Vegetable oils	j=1 Olive oil, virgin	11416	15806	223.16
i=5 Vegetables	j=1 Tomatoes	0	0	0.00
	j=2 Peas	0	0	0.00
i=6 Fruits	j=1 Oranges	0	0	0.00
	j=2 Bananas	0	0	0.00
i=7 Meat	j=1 Beef and veal	15409	28325	1401.64
	j=2 Chicken meat	4325	7628	1401.64
i=8 Dairy	j=1 Cow milk	1021	2470	411.43
	j=2 Chicken eggs	3265	5013	0.00

APPENDIX D: MODEL DECISION VARIABLES AND CONSTRAINTS

Table 21: List of model decision variables

Name	***Expression***	***Type***	***Number***	***Unit***
Food Consumption	X_{ij}	Primary	$\sum_{i=1}^{I} J(i)$	g/cap/day
Food Demand	D_{ij}	Auxiliary	$\sum_{i=1}^{I} J(i)$	ton/yr
Food Production	P_{ij}	Primary	$\sum_{i=1}^{I} J(i)$	ton/yr
Food Import, Export	IMP_{ij}, EXP_{ij}	Primary	$\sum_{i=1}^{I} J(i)$ each	ton/yr
Crop Demand	D_{mn}	Auxiliary	$\sum_{m=1}^{M} N(m)$	ton/yr
Crop production	P_{mndrsq}	Primary	$DRSQ \sum_{m=1}^{M} N(m)$	ton/yr
Crop production (district)	P_{mnd}	Auxiliary	$D \sum_{m=1}^{M} N(m)$	ton/yr
Crop production (national)	P_{mn}	Auxiliary	$\sum_{m=1}^{M} N(m)$	ton/yr
Crop Import, Export	IMP_{mn}, EXP_{mn}	Primary	$\sum_{m=1}^{M} N(m)$	ton/yr
Feed Demand	$D_{i'j'}$	Auxiliary	$\sum_{i'=1}^{I'} J'(i')$	ton/yr
Feed Production	$P_{i'j'}$	Primary	$\sum_{i'=1}^{I'} J'(i')$	ton/yr
Feed Import, Export	$IMP_{i'j'}$, $EXP_{i'j'}$	Primary	$\sum_{i'=1}^{I'} J'(i')$ each	ton/yr
Livestock Demand	$D_{m'n'}$	Auxiliary	$\sum_{m'=1}^{M'} N'(m')$	animal/yr
Livestock Production	$P_{m'n'}$,	Primary	$\sum_{m'=1}^{M'} N'(m')$	animal/yr
Livestock Import, Export	$IMP_{m'n'}$, $IMP_{m'n'}$	Primary	$\sum_{m'=1}^{M'} N'(m')$ each	animal/yr

Table 21 (continued): List of model decision variables

Name	***Expression***	***Type***	***Number***	***Unit***
Fertilizer Demand	$D\_N_{FER,mndrsq}$	Primary	$DRSQ\sum_{m=1}^{M} N(m)$	kgN/ha
Manure Demand	$D\_N_{MAN,mndrsq}$	Primary	$DRSQ\sum_{m=1}^{M} N(m)$	kgN/ha
Fertilizer Demand (National)	$D_{N_{FER}}$	Auxiliary	1	kgN/yr
Fertilizer Production	$P_{N_{FER}}$	Primary	1	kgN/yr
Fertilizer Import, Export	IMP_N_{FER}, EXP_N_{FER}	Primary	2	kgN/yr
Manure Demand (National)	$D_{N_{MAN}}$	Auxiliary	1	kgN/yr
Manure Production	$P_{N_{MAN}}$	Auxiliary	1	kgN/yr
Manure Import, Export	IMP_N_{MAN}, EXP_N_{MAN}	Primary	2	kgN/yr
Water Production	$P_{u,v,w}$	Primary	UVW	m^3/yr
Energy Carrier Demand	D_g	Auxiliary	G	kWh/yr
Energy Carrier Production	$P_{ef,g}$	Primary	$G\sum_{e=1}^{E} F(e)$	kWh/yr
Energy Carrier Production (national)	P_g	Auxiliary	G	kWh/yr
Energy Carrier Import, Export	IMP_g, EXP_g	Primary	G each	kWh/yr
Energy Source Demand	D_e	Auxiliary	E	Raw source/yr
Energy Source Production	P_e	Primary	E	Raw source/yr
Energy Source Import, Export	$IMP_e,\ EXP_e$	Primary	E each	Raw source/yr

Table 22: List of model constraints

Name		***Equation***	***Variables***
Balance Constraints	*Food*	$P_{ij} + IMP_{ij} - EXP_{ij} = D_{ij}$	i & j
		$D_{ij} = \dfrac{X_{ij} * population * 365.25}{10^6 * \left(1 - waste\ factor_{ij}\right)\left(1 - loss\ ratio_{ij}\right)}$	i & j
	Feed	$P_{i'j'} + IMP_{i'j'} - EXP_{i'j'} = D_{i'j'}$	i' & j'
	Crop	$P_{mn} + IMP_{mn} - EXP_{mn} = D_{mn}$	m & n
		$(D_{mn}) = A \times (P_{ij}) + A' \times (P_{i'j'})$	m, n, i, j, i', j'
		$P_{mn} = \sum_{d=1}^{D} P_{mnd}$	m, n, d
		$P_{mnd} = \sum_{r=1}^{R} \sum_{s=1}^{S} \sum_{d=1}^{D} P_{mndrsq}$	m, n, d, r, s, q
	Livestock and Feed	$P_{m'n'} + IMP_{m'n'} - EXP_{m'n'} = D_{m'n'}$	m' & n'
		$D_{i'j'} = \sum_{m'=1}^{M'} \sum_{n'=1}^{N'} \left(X_{i'j',m'n'} * Livestock\ population_{m'n'}\right)$	i', j', m', n'
	Fertilizer & Manure	$P\_N_{FER} + IMP\_N_{FER} - EXP\_N_{FER} = D\_N_{FER}$	-
		$P\_N_{MAN} + IMP\_N_{MAN} - EXP\_N_{MAN} = D\_N_{MAN}$	-

Table 22 (continued): List of model constraints

Name		***Equation***	***Variables***
Balance Constraints	*National Fertilizer & Manure Demand*	$D\_N_{FER} = \sum_{m=1}^{M}\sum_{n=1}^{N(m)}\sum_{d=1}^{D}\sum_{r=1}^{R}\sum_{s=1}^{S}\sum_{q=1}^{Q} D\_N_{FER,mndrsq}$	m, n, d, r, s, q
		$D\_N_{MAN} = \sum_{m=1}^{M}\sum_{n=1}^{N(m)}\sum_{d=1}^{D}\sum_{r=1}^{R}\sum_{s=1}^{S}\sum_{q=1}^{Q} D\_N_{MAN,mndrsq}$	m, n, d, r, s, q
	Energy	$P_e + IMP_e - EXP_e = D_e$	e
		$P_g + IMP_g - EXP_g = D_g$	g
		$P_g = \sum_{e=1}^{E}\sum_{f=1}^{F} P_{efg}$	e, f, g
	Water	$P_u = \sum_{v=1}^{V}\sum_{w=1}^{W} P_{uvw}$	u, v, w
	Land	$\frac{P_{mndrsq}}{PYIELD_{mn}} = CL_{mndrsq}$	m, n, d, r, s, q
		$\sum_{m=1}^{M}\sum_{n=1}^{N(m)}\sum_{d=1}^{D}\sum_{r=1}^{R}\sum_{s=1}^{S}\sum_{q=1}^{Q} CL_{mndrsq} = TCL$	m, n, d, r, s, q

Table 22 (continued): List of model constraints

Name		***Equation***	***Variables***
Nutritional Constraints		$L_k \leq \sum_{i=1}^{I}\sum_{j=1}^{J(i)} \frac{NTR_{ijk}}{100} * \left(Edible\ portion\ of\ X_{ij}\right) \leq U_k$	i, j, k
Manure Production Constraints		$N\_EX = \sum_{m'=1}^{M'}\sum_{n'=1}^{N'(m')} (Livestock\ excretion_{m'n'} \times\ Livestock\ population_{m'n'})$	m', n'
		$P\_N_{MAN} = N\_EX * (1 - \Delta)$	-
Planetary Boundary Constraints		$\frac{Total\ natural\ N\ fixation\ +\ Total\ added\ N}{Population} \leq\ per\ capita\ N\ fixation\ planetary\ boundary$	-
Resource Constraints	*Land*	$TCL +\ Land\ for\ energy\ production\ \leq Total\ available\ land$	-
	Energy	$P_e\ \leq\ Available\ energy\ sources$	e
	Water	$P_u\ \leq\ Available\ water\ resources$	u