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Incorporating nitrogen in the water-energy-food nexus: An optimization approach



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ABSTRACT

Growing populations and improved standards of living are increasing the global demand for food. Having to meet these demands, agricultural systems imposed unprecedented stress on water, land, energy and nutrient cycling on all scales. With nitrogen being a limiting factor for plant growth, intensified application of nitrogen fertilizers was necessary to meet the growing crop yield targets in food production, causing excessive quantities of reactive nitrogen to enter our ecosystem resulting in detrimental effects on the environment and human health. As such, this work develops a mathematical optimization model for nitrogen allocation under sustainable water, food and energy security targets, with nitrogen use efficiency as a primary indicator, and the nitrogen planetary boundary as a primary environmental constraint. Additional nutritional, socioeconomic and natural resources constraints are included. The model incorporates the nitrogen cycle within the land-crop-food continuum and optimizes the nitrogen footprint required to meet food demands, while accounting for water, energy and carbon footprints. A hypothetical case study validates the model and examines the sensitivity of the nexus to nitrogen input and nitrogen use efficiency, under different nitrogen, water and land availability scenarios and different nitrogen use efficiency and nitrogen input policy targets. The results indicate that the dynamics of the water-energy-food (WEF) nexus are highly sensitive to nitrogen. This work emphasizes the potential role of nitrogen as a primary decision factor when addressing WEF security and sustainability in agricultural systems, particularly when setting agricultural policies.

1. Introduction

Nitrogen (N) plays an indispensable role in food security as a limiting nutrient for crop growth. To cope with growing populations and 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, causing environmental drawbacks from excessive inputs of 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 results in increased rates of ammonia volatilization and higher nitrous oxide (N₂O) emissions, both contributors to climate change. Nitrate production alone is a source of high nitrous oxide emissions (Woods et al., 2010). Nitrogen fertilizers are also

responsible for excessive leaching of nitrates (NO₃⁻) and nitrites (NO₂⁻) to water bodies, causing algal blooms, eutrophication, and in extreme situations, development of "dead zones". Aside from agriculture, nitrogen is a primary by-product of the energy and transport industries. N₂O and NO_x emissions from fossil fuel combustion are greenhouse gasses (GHGs) contributing to ozone depletion and global warming. From an energy standpoint, food systems as a whole account for 30% of global energy consumption (Batlle-Bayer et al., 2020), and the fertilizer industry accounts for 50% of agricultural energy requirements (Woods et al., 2010) and 1.2% of the global energy consumption (Swaminathan and Sukalac, 2004).

This discussion leads to two main observations. The first is that the effects of excessive reactive nitrogen input evolve when shifting from a local scale perspective to a global one (Galloway et al., 2003). This is what makes the nitrogen biogeochemical cycle an "aggregated" process, meaning that in addition to their direct effect on immediate ecosys-

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Fig. 1. The broad model framework.

tems, nitrogen compounds also pose a threat to overall environmental resilience (Sutton et al., 2013). This was highlighted in 2009 when the planetary boundaries concept was first introduced. The biogeochemical cycles of nitrogen and phosphorus were recognized to have planetary boundaries, with research indicating that their thresholds had already been exceeded (Rockström et al., 2009b; Steffen et al., 2015). The second observation is that nitrogen is interlinked to all three sectors of water, energy and food. Nitrogen's ability to boost agricultural yields makes it integral to food security, while its natural presence in fossil fuels and corresponding footprint from biofuel production makes it indispensable to energy security. Meanwhile, its polluting effect ties it well with water security and climate change.

This interlinkage can be best assessed by incorporating nitrogen as a fourth pillar to the Water-Energy-Food Nexus (WEF nexus) framework (Higgins and Abou Najm, 2020; Hoff, 2011). The WEF nexus has appeared in the literature as an emerging framework for resource management and environmental assessment. However, the literature that takes nutrients, specifically nitrogen, into consideration is very limited. Fernandez-Rios et al. (2021) conduct a review on the inclusion of nutrient profiles within WEF nexus modeling, but little work includes nitrogen specifically. This is not to say that studies do not highlight the importance of nitrogen with the WEF nexus framework. Davidson et al. (2016) discuss the importance of incorporating nitrogen management into the nexus and demonstrate its impact using two specific case studies. Similarly, Hua et al. (2020) highlight the importance of including nitrogen, among other nutrients and footprint, as a priority biophysical indicator of the WEF nexus to respect planetary boundaries.

While some studies do directly include nitrogen in WEF nexus assessment, it is usually within a very specific context. Villarroel Walker et al. (2014) applied multi-sectoral analysis to estimate resources (water, energy, and nutrients including nitrogen) and fluxes across five sectors (water, energy, waste, food, and forestry). Ibarrola-Rivas and Nonhebel (2016) focused on the nexus of land, food, and nitrogen fertilizer for an integrated assessment of agricultural resources impact on food production. Liu et al. (2016) studied nitrogen flows on a global scale, including embedded nitrogen in trade, and assessed its role in meeting the hunger eradication targets set by the United Nations Millennium Development Goals. Conijn et al. (2018 presented a similar study but set planetary boundaries as the primary constraint. Mortensen et al. (2016) accounted for nitrogen flow in arid river corridors within a WEF context. Yao et al. (2018) modelled nutrient flow in a local food energy water system and simulates nitrogen flows and stocks to study the impact on crop production, energy technology selection, and nutrient management. Li et al. (2021) put forth a relative WEF nexus index to evaluate the synergy of the WEF nexus within cropping systems, and accounts for nitrogen input from fertilizer. On a more comprehensive level, Wen et al. (2021) simulate the general water-energy-nutrient nexus by applying substance flow analysis (SFA) to develop a multi-sectoral metabolism analysis model for the metabolism of nutrients (carbon, nitrogen, and phosphorous), water and energy across five sectors: water, waste, livestock husbandry, forestry, and residential. Thus, there remains an explicit lack of nitrogen inclusion within the WEF nexus as a whole.

Recognizing the need for explicit coupling between the cycling of major biogeochemical elements (particularly nitrogen, carbon and phosphorous) and the nexus, this work presents an optimization model that establishes the relations between nitrogen and the Water-Energy-Food nexus. The work is based on the models developed by Mortada et al. (2018) and Chamas et al. (2021) but goes further to incorporate the nitrogen cycle into the generalized model, setting the nitrogen fixation planetary boundary as a fundamental constraint, and using Nitrogen Use Efficiency (NUE) as a primary indicator. The model uses available natural resources and regional WEF demands to optimize nitrogen use and resource allocation under different objective functions and constraints (Fig. 1). Being a multi-scale problem, the model allows for nutrient tracking and management from farm to global scales while optimizing nitrogen policies that satisfy WEF demands. In addition, the model facilitates policy comparison when considering different nitrogen indicators (nitrogen use efficiency versus nitrogen input for example), behavioural dietary changes, or sustaining regional self-sufficiency in food and energy production and consumption.

2. Theory and model formulation

The model attempts to capture the most significant nitrogen flows within the water, energy and food sectors by identifying the trade-offs between the nexus and the natural nitrogen cycle and the effects of anthropogenic activities on the environment and nexus.



Fig. 2. The terrestrial nitrogen cycle and the anthropogenic contribution.



Nitrogen Output

Fig. 3. Nitrogen budget components adopted in the model.

2.1. Nitrogen

2.1.1. The terrestrial nitrogen cycle

The nitrogen cycle is summarized in Fig. 2, showing that nitrogen comes in different forms across various environmental compartments. 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 caused higher loss rates. The consequence was the accumulation of reactive nitrogen at specific locations in amounts beyond what the natural ecosystem could accommodate for, resulting in the detrimental effects of increased N₂O and NH₃ emissions or nitrate leaching (Galloway et al., 2003; Reay, 2015).

2.1.2. Nitrogen use efficiency

In simple terms, nitrogen use efficiency (NUE) is a ratio of nitrogen outputs to nitrogen inputs within an agricultural system. More details on NUE definitions across operational scales is in the supplementary material (Table S1). The scale flexibility of our model allows us to evaluate NUE at different levels. This work assesses NUE at a plot scale, for specifically defined soil, crop, weather, and management conditions. The overall NUE is based on a farm-gate budget, accounting for both agriculture and livestock. Nitrogen efficiency can also be studied at the regional/global level accounting for import and export of goods as well (nitrogen trade). At the plot level, the main natural nitrogen inputs are: i) biological nitrogen fixation, ii) atmospheric deposition, iii) nitrogen available in soil (from biological and nonsymbiotic nitrogen fixation), and iv) added agricultural inputs of nitrogen in the form of synthetic fertilizers and applied manure. N output is nitrogen content removed with yielded crops, which accounts for harvested, fodder, and grazing crops. Crop residues are considered lost N. Assuming steady state and a one-year span (or one cropping season), soil N changes are accounted for but not deemed significant. Nitrogen not taken up by the plant can be lost either through denitrification and gaseous emissions (N₂, N₂O, NO), ammonia volatilization, or nitrate leaching. Moving from plot to farm budget, livestock components are added, such that feed intake is input and animal products are output. Excreted nitrogen from livestock is used to calculate locally available manure. The adopted farm budget nitrogen cycle is illustrated in Fig. 3.

2.2. Model framework

Figure 4 presents a flowchart showing model connections and the incorporation of nitrogen into the three nexus pillars of water, energy, and food. Shaded tabs represent the model's primary decision variables (see Table 2 for details). 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



Fig. 4. Model Flowchart.

or national level, but has the flexibility to assess different dimensions and region sizes. Temporally, the model also operates at fine resolution (weeks to months) for dynamic processes (irrigation and fertilization) and aggregates to larger temporal scale (season to year) for other systems components, such as nutrient cycling, cropping seasons, livestock production, and national water, energy and food policies (demand, production, import and export). A year-to-year balance is adopted to accommodate for the opposite ends of the time scale.

2.2.1. Decision variables

Nitrogen decision variables are expressed with synthetic nitrogen fertilizer and manure. Water decision variables encompass withdrawal source, treatment, and end use as water allocations. Similarly, energy variables are listed as function of primary source, processing technology, and final energy carrier. Energy and water components of this model are discussed in more detail by Chamas et al. (2021). Primary decision variables are those expressed at the smallest scale (crop, climate, soil, and irrigation conditions level). Auxiliary decision variables are added

to link between different scales of the model. The model decision variables are summarized in Table 1.

2.2.2. Objective functions (OF)

Here, we present two variations of possible objective functions along with their advantages and disadvantages.

2.2.2.1. OF 1: Maximizing NUE. The central objective of the nitrogen problem is maximizing NUE for optimal nitrogen usage (Eq. (1)) by meeting production demands while minimizing nitrogen losses. Alone, this will favor the use of crops with low nitrogen requirements and high removal rates and discourage nitrogen inefficient animal products (which can be balanced with added constraints on diet preferences and recommended guidelines).

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

NUE over the whole system is calculated as shown in Eq. (2). Nitrogen outputs ($N_{outputs}$) represent nitrogen yield from crop and animal

Table 1

Model decision variables.

Variable	Unit	Definition	Variable	Unit	Definition
BNF _{mndrsq}	kgN/ha	Biological nitrogen fixation for crop n in crop group m grown in district d having climate r with soil s using irrigation technique q	$IMP_{i'j'}$	ton/year	Import quantity of feed item j' in feed group i'
CL_{mndrsq}	ha	Land cultivated growing crop n in crop group m grown in district d having climate r with soil s using irritation technique q	IMP _{mn}	ton/year	Import quantity of crop n in crop group m
D _e	unit of <i>e</i>	Domestic demand quantity of energy source e	$IMP_{m'n'}$	head/year	Import quantity of livestock group m' in livestock type n'
D_{a}	unit of g	Domestic demand quantity of energy form g	IMP N _{FFP}	kgN/year	Import quantity of nitrogen fertilizer
D_{ij}^{s}	ton/year	Domestic demand quantity of food item <i>j</i> in food	IMP_N _{MAN}	kgN/year	Import quantity of nitrogen from manure
$D_{i'j'}$	ton/year	Domestic demand quantity of feed item j' in feed	$N_EX_{MAN,m'n'}$	kgN/year	Excretion quantity of manure from livestock group w' in livestock type v'
D _{mn}	ton/year	Domestic demand of crop <i>n</i> in crop group <i>m</i>	$NDEP_{mndrsq}$	kgN/ha	Nitrogen deposition for crop n in crop group m grown in district d having climate r with soil s
					using irrigation technique q
$D_{m'n'}$	head/year	Domestic demand quantity of livestock group m' in livestock type n'	N D _{mndrsq}	kgN/year	Nitrogen demand for crop <i>n</i> in crop group <i>m</i> grown in district <i>d</i> having climate <i>r</i> with soil <i>s</i> using irrigation technique <i>q</i>
D_u	m ³ /year	Domestic demand quantity of water from source <i>u</i>	N_REQ_{mndrsq}	kgN/year	Nitrogen requirement for $\operatorname{crop} n$ in $\operatorname{crop} \operatorname{group} m$ grown in district <i>d</i> having climate <i>r</i> with soil <i>s</i>
D_v	m ³ /year	Domestic demand quantity of water for use v	NSF_{mndrsq}	kgN/ha	Nonsymbiotic nitrogen fixation for crop n in crop group m grown in district d having climate r with soil s using irrigation technique a
DN	kaN/woor	Demand quantity of nitrogen fortilizer	D N	kaN/waar	Broduction quantity of nitrogen fertilizer
D_{NFER} $D_N_{FER,mndrsq}$	kgN/ha	Demand quantity of introgen fertilizer Demand quantity of nitrogen fertilizer for crop n in crop group m grown in district d having climate r with soil s using irrigation technique q	P_N_{MAN}	kgN/year	Production quantity of manure nitrogen
D_N_{MAN}	kgN/year	Demand quantity of manure nitrogen	$P_N_{MAN,m'n'}$	kgN/year	Production quantity of manure nitrogen from livestock group m' in livestock type n'
$D_N_{MAN,mndrsq}$	kgN/ha	Demand quantity of manure nitrogen for crop <i>n</i> in crop group <i>m</i> grown in district <i>d</i> having	P_e	(unit of e)/year	Production quantity of energy source <i>e</i>
EXP_{e}	unit of <i>e</i>	Export quantity of energy source e	P_{efg}	(unit of g)/year	Production quantity of energy form g from source e using technology f
EXP	unit of a	Export quantity of energy source g	Р	(unit of g)/year	Production quantity of energy source g
EXP_{ij}	ton/year	Export quantity of food item j in food group i	P_{ij}	ton/year	Production quantity of food item <i>j</i> in food group
$EXP_{i'j'}$	ton/year	Export quantity of feed item j' in feed group i'	$P_{i'j'}$	ton/year	Production quantity of feed item j' in feed group i'
EXP	ton/year	Export quantity of crop n in crop group m	Р	ton/year	Production quantity of crop n in crop group m
$EXP_{m'n'}$	head/year	Export quantity of livestock group m' in livestock type n'	P _{mndrsq}	ton/year	Production quantity of crop n in crop group m grown in district d having climate r with soil s using irritation technique a
EXP_N_{FER}	kgN/year	Export quantity of nitrogen fertilizer	$P_{m'n'}$	head/year	Production quantity of livestock group m' in livestock type n'
EXP_N_{MAN}	kgN/year	Export quantity of manure nitrogen	P_{uvw}	m ³ /year	Production quantity of water from source u for use/quality v using technology w
IMP	unit of e	Import quantity of energy source e	PYIELD	ton/ha	Potential crop yield of crop <i>n</i> in crop group <i>m</i>
IMPa	unit of g	Import quantity of energy source g	TAL	ha	Total available land
IMP_{ii}^{s}	ton/year	Import quantity of food item <i>j</i> in food group <i>i</i>	TCL	ha	Total cultivated land
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products combined and summed over all considered system characteristics: districts (*d*) in climates (*r*) with soil textures (*s*) under irrigation techniques (*q*). $N_{inputs,crops}$ represent the natural and added nitrogen to crops from fixation (biological, BNF, and nonsymbiotic, NSF), deposition (NDEP), fertilizers and manure. $N_{inputs,animals}$ represent the intake of nitrogen from feed consumption. Segmenting inputs and outputs into crop and animal components allows for the computation of each of their respective efficiencies separately. However, care should be taken when calculating the overall efficiency NUE to make sure that no nitrogen input or output is double counted. Detailed calculations of the input and output components are available in supplementary material.

$$NUE = \frac{N_{outputs}}{N_{inputs}} = \frac{N_{outputs, \ crops} + N_{outputs, \ animals}}{N_{inputs, \ crops} + N_{inputs, \ animals}}$$
(2)

2.2.2.2. OF 2: Minimizing nitrogen consumption per capita. While NUE is an excellent indicator of nitrogen use, it does not give any idea on the

magnitude of nitrogen applied or lost. Even with high NUE values, the quantities of nitrogen lost to or consumed by a specific ecosystem can still be detrimental, if originating from excessive original nitrogen input. Thus, nitrogen input value is used to evaluate nitrogen inputs per capita to satisfy dietary demands, then aggregated up to regional or national status of nitrogen use for evaluation against the planetary boundary on nitrogen.

This objective function seeks to minimize nitrogen consumption per capita. This consumption value is calculated from two source types: natural (deposition: NDEP, biological fixation: BNF, and nonsymbiotic fixation: NSF) and added (fertilizer: D_NFER , and manure: D_NMAN). The natural nitrogen sources are summed across crop groups (*m*), crop types (*n*), districts (*d*), climates (*r*), soil types (*s*), and irrigation techniques (*q*) for a comprehensive value.

$$OF(2) = Min\left(N_{consumption, capita}\right) = Min\left(\frac{N_{natural} + N_{added}}{population}\right)$$
(3)

where:

$$N_{natural} = \sum_{m=1}^{M} \sum_{n=1}^{N(m)} \sum_{d=1}^{D} \sum_{r=1}^{R} \sum_{s=1}^{S} \sum_{q=1}^{Q} \left(NDEP_{mndrsq} + BNF_{mndrsq} + NSF_{mndrsq} \right)$$
(4)

$$N_{added} = D_N_{FER} + D_N_{MAN} \tag{5}$$

This problem will favor 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 compared to the introduction of external sources such as synthetic fertilizers.

2.2.3. Constraints

The model constraints cover all nexus resources (water, energy, food, land) as detailed in Mortada et al. (2018) in addition to ones covering feed, livestock, nitrogen fertilizer, manure, and planetary boundaries, as pertains to this work. More details on the mathematical formulation of equations capturing demand and production calculations for food, feed, and crops are in the supplementary information.

2.2.3.3. Balance constraints. This section provides an overview of the balance constraints imposed on food, feed, livestock, and crops. The national balance (*D*) ensures that domestic demand is satisfied from local production (*P*) and imports (*I M P*), while accounting for exports (*E X P* and assuming no stock inventory changes. This applies to food item *j* in food group *i* (Eq. (6)), feed item *j'* in feed group *i'* (Eq. (7)), crop type *n* in crop group *m* (Eq. (8))., and livestock type *n'* in livestock group *m'* (Eq. (9)).

$$P_{ij} + IMP_{ij} - EXP_{ij} = D_{ij} \forall i \& j$$
⁽⁶⁾

$$P_{i'j'} + IMP_{i'j'} - EXP_{i'j'} = D_{i'j'} \forall i' \& j'$$
(7)

$$P_{mn} + IMP_{mn} - EXP_{mn} = D_{mn}\forall m, n \tag{8}$$

$$P_{m'n'} + IMP_{m'n'} - EXP_{m'n'} = D_{m'n'} \forall m', n'$$
(9)

2.2.3.4. Nutritional intake constraint. It is important to note that nutrients within consumed food must meet specific standards for it to be deemed of acceptable nutritional quality for a basic diet. The amount of nutrient k in 100 gs of consumed food X_{ij} (denoted as $\frac{NTR_{ijk}}{100}$) must fall between a lower (L_k) and upper (U_k) limit. These limits are obtained from international databases such as the WHO and FAO. This constraint is expressed in the following equation.

$$L_k \le \sum_{i=1}^{I} \sum_{j=1}^{J(i)} \frac{NTR_{ijk}}{100} * X_{ij} \le U_k$$
(10)

2.2.3.5. Livestock-manure constraints. From the available livestock population, it is possible to compute the potential for local manure production from livestock excretions. Manure produced $(P_N_{MAN,m'n'})$ is calculated from livestock excretions $(N_E X_{m'n'})$, excluding the fractions lost in other processes for each livestock type $(\Delta_{m'n'})$. IPCC calculations are used to 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, notated by Δ (IPCC 2006). Values for Δ are available in the supplementary material (Table S2). Total manure production (P_N_{MAN}) is then calculated as the summation of $P_N_{MAN,m'n'}$ across livestock types and groups.

$$P_{N_{MAN,m'n'}} = N_{EX_{MAN,m'n'}} * (1 - \Delta_{m'n'})$$
(11)

2.2.3.6. Nitrogen requirement constraints. Nitrogen requirements $(N_REQ_{mndrsq} \text{ in kgN/ha})$ for crop *n* in crop group *m* grown in district *d* having climate *r* with soil *s* using irrigation technique *q* is the amount of nutrient nitrogen needed for optimal crop growth, below which nitrogen becomes a limiting factor for this growth. Nitrogen demand (ND_{mndrsq}) quantifies needed nitrogen that can be supplied from either fertilizers $(D_N_{FER,mndrsq})$ or manure $(D_N_{MAN,mndrsq})$ for each crop *n* in crop group *m* grown in district *d* having climate *r* with soil *s* using irrigation technique *q*, as in the following equation. It is noted that nitrogen demand values can be obtained from the FAO (2003).

$$ND_{mndrsq} = D_N_{FER,mndrsq} + D_N_{MAN,mndrsq}$$
(12)

Nitrogen demand (ND_{mndrsq}) supplements the natural nitrogen sources in the form of nitrogen deposition $(NDEP_{mndrsq})$, biological nitrogen fixation (BNF_{mndrsq}) , and nonsymbiotic fixation (NSF_{mndrsq}) . These values are crop specific based on growth conditions (in district *d* having climate *r* with soil *s* using irrigation technique *q*). As such, the nitrogen demand (ND_{mndrsq}) is determined by subtracting the sum of these natural inputs from the amount of nitrogen required for optimal growth $(N_{REQmndrsq})$.

$$ND_{mndrsq} = N_{REQ_{mndrsq}} - \left(NDEP_{mndrsq} + BNF_{mndrsq} + NSF_{mndrsq}\right)$$
(13)

2.2.3.7. Fertilizer and manure nitrogen national balance constraints. Manure and fertilizer demand are satisfied from the production, import and export of each. National fertilizer $(D_N _{FER})$ and manure $(D_N _{MAN})$ are calculated by adding all fertilizer and manure requirements for each crop across all growth conditions, respectively. The national balances, as described above, for fertilizer and manure nitrogen are shown in Eqs. (14) and (15).

$$P_N_{FER} + IMP_N_{FER} - EXP_N_{FER} = D_N_{FER}$$
(14)

$$P_N_{MAN} + IMP_N_{MAN} - EXP_N_{MAN} = D_N_{MAN}$$
(15)

2.2.3.8. Planetary boundary on nitrogen fixation. The planetary boundary on nitrogen fixation refers to a cut off nitrogen value (currently 62 Tg N per year, O'Neill et al., 2018), beyond which additional nitrogen increases the risk of abrupt and possibly irreversible climate change (Rockström et al., 2009a). The total fixation limit covers nitrogen for all uses, agricultural or industrial, and includes both natural nitrogen fixation (deposition, biological fixation, and nonsymbiotic fixation in Eq. (7)) and added nitrogen (in the form of fertilizer and manure in Eq. (8)). For analytical purposes, the total fixation limit is converted to a per capita basis, coming to 8.9 kgN/capita/year (O'Neill et al., 2018). This value is derived from a cumulative value of total nitrogen (natural or added) allowed on an annual basis globally, hence it is known as a planetary boundary. Crossing this threshold increases the risk of abrupt or irreversible environmental change. As such, the constraint on nitrogen fixation per capita is expressed as follows, and should be less than nitrogen fixation allocated per capita for the planetary boundary $(N_{fixation, planetary, capita}).$

$$\frac{Total \ natural \ N \ fixation \ + \ Total \ added \ N}{Population} \le N_{fixation, planetary, capita}$$
(16)

However, it is important to quantify nitrogen flows into croplands to assess nitrogen stress and scarcity levels, which in the long run can affect yields, poverty, food insecurity, and malnutrition (Liu et al., 2010). Table 2 presents the ranges of nitrogen flow into cropland and categorizes the nitrogen stress level accordingly.

It is noted that the values in Table 2 differ from the allocated planetary boundary limit, in that they only represent flow into cropland to determine whether there is enough nitrogen for sufficient crop growth. On the other hand, the planetary boundary limit represents a net value, Table 2

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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	

accounting for input, output, transformation, and losses for all sources of nitrogen across different compartments.

2.2.3.9. Water and energy constraints. Having addressed the food sector, which is more directly associated with nitrogen, the remaining constraints address the water, energy, and land sectors. For the water sector, the total amount of water produced (P_u) must not exceed the amount of available water resources. P_u is calculated from the summation of water production (P_{uvuv}) from source *u* for end use *v* using technology *w* across all considered end uses and sources.

$$P_u = \sum_{v=1}^{V} \sum_{w=1}^{W} P_{uvw}$$
(17)

Similarly, the total amount of energy produced (P_e) must not exceed the amount of available energy resources. Balances are performed on energy sources (e) and energy carriers (g), such that demand is equal to production plus imports minus exports.

$$P_e + IMP_e - EXP_e = D_e \tag{18}$$

$$P_g + IMP_g - EXP_g = D_g \tag{19}$$

Total energy carrier production (P_g) is computed from the summation of the production of energy carrier *g* from energy source *e* applying technology *f* across all considered energy sources and carriers.

$$P_g = \sum_{e=1}^{E} \sum_{f=1}^{F} P_{efg}$$
(20)

2.2.3.10. Land constraints. In terms of land, the basic constraint is that amount of land used for food (TCL: total cultivated land) and energy production must be less than the total available land (TAL).

$$TCL + Land for energy production \leq TAL$$
 (21)

Other parameters like reserves and domestic, recreational, and other forms of land use can be added to this equation. Furthermore, the quantity of cultivated land per crop (CL_{mndrsq}) is calculated from P_{mndrsq} (production of crop (m, n) in district *d* in climate *r* with soil *s* using irrigation technique *q*) divided by the potential yield of the crop $(PYIELD_{mn})$. In turn, *TCL* is obtained from the summation of CL_{mndrsq} over the different irrigation techniques, soil types, climate types, districts, and crops.

$$TCL = \sum_{m=1}^{M} \sum_{n=1}^{N(m)} \sum_{d=1}^{D} \sum_{r=1}^{R} \sum_{s=1}^{S} \sum_{q=1}^{Q} CL_{mndrsq} = \sum_{m=1}^{M} \sum_{n=1}^{N(m)} \sum_{d=1}^{D} \sum_{r=1}^{R} \sum_{s=1}^{S} \sum_{q=1}^{Q} \frac{P_{mndrsq}}{PYIELD_{mn}}$$
(22)

2.2.3.11. Non-negativity constraints. All decision variables are non-negative.

3. Model validation with hypothetical case study

3.1. Case study description

To validate our model and test the proposed objective functions, a generic hypothetical case study is evaluated (Fig. 5). One district d, consisting of two climate types to provide the model with more options to

choose from. The climates determine the water footprints of the specified crops, so we chose the global average and MENA (Middle East and North Africa) climates to represent wet and dry climates, respectively. For soils and irrigation, we assumed one soil texture (fixed as silty clay loam) and two irrigation techniques (sprinkler irrigation and drip irrigation) characterized by different water efficiencies.

As for crops, nine agricultural crops are included in the analysis, in addition to two fodder crops. Two basic livestock groups, cattle and poultry, are also included. For simplicity, three food components are accounted for: water, proteins, and calories. Crops were selected based on their ability to provide options for multiple fair diets, accounting for variations in nutrient content, yields, as well as land, water, nitrogen, and energy footprints. There is a total of thirteen food items, plus drinking water.

Nitrogen requirements for each crop are calculated and verified with data from the literature and common farmer practices (FAO, 2003). We assumed that yields, nitrogen requirements, and energy footprints of crops, livestock, food and feed items are similar across the two climates, with values equal to that of the global average (Climate 1). Only crop water footprints are calculated for each climate separately, but all crops can be grown in both climates. It is assumed that each climate type covers half of the total available land area. Nitrogen requirements are compared against the water, energy and land (yield) footprints of the crops for more detailed analysis under different scenarios. The supplementary material contains the case study data for all the model components.

It is noted that the model does not consider irrigation water as a source of nitrogen. In addition, the model assumes that manure nitrogen losses are lower than with synthetic fertilizer for two reasons: i) only some of the nitrogen in manure is readily available to plants and this available nitrogen is prone to loss, and ii) synthetic fertilizer renders nitrogen immediately available to plants, whereas nitrogen in manure is released over time (Mehata et al., 2017).

In summary, the developed case study compiles 214 decision variables and 228 constraints. Objective functions, OF (1) and OF (2), are assessed to evaluate the food security and nitrogen status of the model. A python script was developed to solve this problem and run sensitivity analysis.

3.2. Adopted approach

Five scenarios were designed to evaluate the proposed model under the two objective functions presented. The first, "Baseline Scenario: Abundant Resources," is a control scenario assuming all resources needed (land, water, energy, and nitrogen) are available and nonlimiting. Working with the two objective functions, this scenario illustrates the difference between targeting a low nitrogen input versus a high nitrogen use efficiency policy. Limitations from available water (Scenario 1), land (Scenario 2) and a decreasing per capita allowable nitrogen application target (Scenario 3) are introduced to assess changes in agricultural policies and resource allocation to ensure food security. In Scenario 4, food security is evaluated at the national level by relaxing self-sufficiency and assess performance with respect to the nitrogen fixation planetary boundary of 8.9 kgN/cap/yr (O'Neill et al., 2018). It is a simple attempt at estimating the ability to sustain self-sufficiency under the suggested planetary boundary policies.

All scenarios with their corresponding variables and studied objective functions are presented in Table 3 below. The nitrogen fixation limit is set to 30 kgN/cap/yr at all times which is the lower threshold for national nitrogen sufficiency level (upper threshold for the "nonitrogen-stress" status), as the aim is to limit affluent nitrogen application (Liu et al., 2010).

Besides the need to ensure a food security status at a national level, the food self-sufficiency ratio, SSR_{ij} is dictated to be equal to or greater than one in all conditions. This is because allowing the food imports will drive the model to import all food items in attempt to decrease local



Fig. 5. Case study description for a population of 100 and total available land of 30 ha, with one soil texture (silty clay loam), two climate types (global/wet and MENA/dry averages) and two irrigation techniques (drip and sprinkler, in different ratios). Three food categories (in green: nine agricultural crops, four animal products, three fodder crops), three nutrients (light green), four water sources (blue), two nitrogen sources (yellow), and one energy form (orange) are considered.

Table 3

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	$30 \rightarrow 0$	30	30
Nitrogen Fixation Limit (kgN/cap/yr)	30	30	30	$30 \rightarrow 0$	30
SSRij = Production/ Demand	≥1	≥1	≥ 1	≥1	$1 \rightarrow 0$
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.

N fixation. In turn, this prevents useful model application and does not allow insightful interpretation of nitrogen use for crop production needs. Therefore, no crop and food item imports are allowed.

4. Results and discussion

4.1. Baseline scenario: Abundant resources

To determine the baseline, initial assessment takes place without any resource limitations and trade policies. It is assumed that there are 30 hectares of cropland, 300,000 m^3 of available water, no limits on energy consumption, and unlimited fertilizer/manure import. With no restrictions on diet preferences and food diversity, the model yields the optimum food choices for the two OFs and their corresponding nitro-

gen and resource consumption while satisfying the primary nutritional constraints of protein and energy requirements. For the purposes of this analysis, a three-tier food consumption system is introduced, where foods consumed in quantities over 200 g/d form the first tier, those consumed in quantities over 100 g/d form the second tier, and the remaining foods form the third tier.

The baseline scenario when maximizing NUE (OF1) provides four first tier foods (maize, potatoes, oranges, and bananas), two second tier foods (wheat and tomatoes), two third tier foods (beans and peas). The diversified diet ensures that the energy and protein constraints are satisfied where the bulk of the protein requirement comes from the wheat and maize. All added nitrogen (1768 kgN/yr) comes in the form of added manure, as the model avoids synthetic fertilizer, due to the lower losses (and thus lower required inputs) of manure compared to fertilizer. This scenario results in an NUE value of approximately 26% corresponding to N consumption value of 21.5 kgN/capita/yr.

The baseline scenario when minimizing nitrogen consumption (OF2) introduces a new food in the second tier: cow milk. This occurs because the model is attempting to minimize the addition of nitrogen in any form (manure or fertilizer) and the best way to do that is to avoid crop cultivation when possible. As such, the model reduces the amount of tomatoes consumed (compared to when maximizing NUE) and turns to cow milk, which comes from dairy cows that have a relatively high nitrogen product to feed efficiency (ratio of nitrogen in product to nitrogen consumed in livestock feed). The peas, tomatoes, and olive oil consumption values are quite low. In the cases of the foods, it improved the overall objective of minimizing nitrogen to have these small amounts consumed (ensuring the satisfaction of nutritional requirements) to avoid adding nitrogen via increased consumption of other foods. Similarly, all added nitrogen (1667 kgN/yr) is in the form of manure. This scenario results in an NUE value of approximately 25% corresponding to N consumption value of 20 kgN/capita/yr.

The difference between NUE and N consumption levels is a tradeoff between the fact that while crops that have high nitrogen removal rates favor an increased NUE, these same crops may require higher nitrogen application to grow (which works against minimizing nitrogen consumption). For example, bean consumption is over 30% higher when maximizing NUE compared to when minimizing Nitrogen consumption. This is because beans are considered a nitrogen efficient crop. On the other hand, cow milk is not consumed in the NUE scenario, because it is more nitrogen efficient to increase consumption in other crop groups than to introduce livestock as a source of nitrogen. Whereas, when minimizing nitrogen consumption, the model opts for cow milk, which does not require any nitrogen application (manure or fertilizer). It is noted that other than cow milk, no livestock product is selected for both objective functions.

4.1.1. Scenario 1: Limited water availability

Beyond the baseline scenario of abundant resources, the first scenario limits water availability to evaluate the sensitivity of NUE and N consumption to water crop and food processing requirements. Model simulations were conducted starting at the abundant limit of $300,000 \text{ m}^3$ of available water, and gradually decreased until no feasible solution could be obtained. The lowest possible amount of water available needs to be approximately 24,095 m³/yr for a feasible solution to both objective functions.

Under OF (1), the model tries to obtain the combination of food items that achieves the highest NUE possible using limited water. As such, it should opt for both water and nitrogen efficient crops. However, given the nutritional constraints, the model is limited in terms of the diet changes that can be made while satisfying the required nutrient consumption. Compared to the baseline scenario, limited water availability drives up the consumption of wheat, negligibly increases the consumption of peas, and decreases the consumption of both oranges and tomatoes. This is because oranges tend to have a high-water requirement, whereas the decreased water availability shifts nutritional value obtained from tomatoes to be extracted from wheat which is indispensable for nutritional requirements and has a lower nitrogen demand. The remaining food items remain relatively consistent.

Under OF (2), the model is expected to select crops that require both low nitrogen and water inputs. This difference in model objective leads to a more distinct changes in diet, where cow milk consumption drops to zero as water availability drops. This is due to the high livestock rearing water requirement for dairy cows. Similarly, orange consumption drops because of its relatively high-water requirements. Wheat and bean consumption increase with decreasing water availability to compensate for the nutritional value lost with the absence of cow milk, tomatoes, and olive oil. Fig. 6 summarizes the results of the limited water availability assessment.

4.1.2. Scenario 2: Limited land availability

Scenario 2 assesses the sensitivity of NUE and N consumption to land availability. In OF (1), it is expected that the model opts for crops that have both high nitrogen removal rates and high yields. In OF (2), the focus is on crops that require less nitrogen input in general. However, these 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. For both objectives, the problem becomes infeasible when land availability drops below 8.4 hectares for OF(1) and 8.2 hectares for OF(2). This difference arises from the premise that total nitrogen application is as dependent on crop yields as it is on crop nutrient requirements. As such, minimizing nitrogen consumption leads the model to immediately opt for the high yield crops thereby initially requiring less land than maximizing NUE. Limited land availability yields similar consumption trends as that of limited water availability.

For OF(1), the same diet composition is obtained until available land exceeds 20 hectares. At this point, the most significant change is the drop in tomato consumption, which is compensated for with slight increases in wheat and peas. The same reasoning as in the limited water scenarios applies. The shift in the amount of manure consumed is minimal (1777 kgN/yr at 30 ha and 1774 kgN/yr).

For OF(2), the point of change is 15 hectares, where orange consumption significantly drops to zero and cow milk and wheat consumption increase. Once again, additional nitrogen comes in the form of manure, with a more noticeable change in application quantities (1725 kgN/yr for cropland area of 8.2 ha and 1671 kgN for cropland area of 30 ha). As the available cropland area decreases the model is forced to increase nitrogen addition to yield the consumption quantities that satisfy nutritional requirements. As the area increases, less manure is needed because more land is available for increased crop growth as opposed to trying to obtain the same amount of growth from a smaller area which would necessitate more added nitrogen due to less available natural nitrogen (from soil). Fig. 7 summarizes the results of the limited land availability assessment.

Across both the water and land analyses, the highest NUE attainable at that limit is 26% and the lowest per capita N consumption is 20 kgN/cap/yr. Both scenarios also indicate that achieving high NUE comes at the expense of high resource use (water and land). However, especially with the limited land scenario, it is important to consider the relation between nitrogen input rates and crop yields to derive more valuable and tangible insight on the land-NUE-N consumption sensitivity.

4.1.3. Scenario 3: Limited per capita nitrogen fixation

Scenario 3 evaluates how high NUE can be maintained under limited nitrogen input conditions. OF (1) is applied starting from the per capita N consumption limit of 30 kgN/cap/yr and gradually decreasing the limit until no feasible solution is obtained. The lowest N consumption limit yielding a feasible solution was 20 kgN/cap/yr, with a corresponding NUE level of 25%, as shown in Fig. 8. This scenario demonstrates that more restricted N consumption limits will hinder the ability of a combination of nitrogen efficient crops to satisfy nutritional demands with, because they also have low nitrogen input requirements (in addition to having high nitrogen removal rates). As such, at the lower limit of 20 kgN/cap/yr, the model opts for the consumption of cow milk instead of tomatoes as discussed above.

As the limit increases to 30 kgN/cap/yr, the model reverses to decrease the consumption of cow milk and increase that of tomatoes, as more nitrogen is allowed into the system. This, not only demonstrates how nitrogen availability affects food choices, but also highlights the need for recycling nitrogen from typically lost sources such as crop residues, BNF, organic wastes, and animal manure. While the addition of new nitrogen to cropland is necessary (due to nitrogen loss in sewage sludge which is not returned to the field), increasing the amount of recycled nitrogen works to decrease the amount of new nitrogen required.



Fig. 6. Water availability analysis showing how diets change (daily consumption) as available water quantity change from a minimum of 24,095m³ to 300,000m³.





4.1.4. How far are we from the nitrogen planetary boundary?

All presented scenarios result in a minimum N consumption rate of 20 kgN/cap/yr, which lies in the range of no nitrogen stress. However, in order to stay within the planetary boundary of nitrogen, a level of no more than 8.9 kgN/cap/yr should be achieved (Steffen et al., 2015). In other words, and to satisfy this constraint, 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. While it is beyond the scope of this study to evaluate those numbers, this study highlights the need for reconciling those ranges between planetary boundary and the suggested ranges of nitrogen flow into cropland (categories of nitrogen stress level in Table 2). Such integration between those two concepts can lead to more efficient nitrogen use while ensuring food security and remaining within the planetary boundaries.

To further analyze this, OF (2) is applied while relaxing the SSR_{ij} limit and allowing for food import until the 8.9 kgN/cap/yr mark is reached. The corresponding SSR_{ij} is approximately 0.44, as shown in Fig. 9. Thus, at the given level of demand, for a local consumption rate of 8.9 kgN/cap/yr, 56% of food demand cannot be locally produced in our specific case study. In other words, 62% of nitrogen demand should be

attained in a sustainable manner as opposed to being inputted into the land each season with the available options we provided to the model. This poses a risky dependency on external sources for food security and reflects how over-exploiting ecosystems to ensure food security eventually cycles to threaten these ecosystems, and consequently, food security once again.

This analysis allows for the conclusion that policy makers should prioritize the achievement of the nitrogen planetary boundary over the use of nitrogen stress level indicators. Using nitrogen stress levels can lead to optimization of the system at the farm level ensuring no nitrogen deficits but prevents the incorporation of broader more realistic considerations that can have global implications. On the other hand, the nitrogen planetary boundary: i) assures environmental continuity, and ii) provides a more accurate reflection of a real-life scenario, where trade considerations must be made.

This conclusion is further reinforced when a multi-objective optimization version of the problem is simulated on the baseline scenario, maximizing NUE and minimizing nitrogen consumption at the same time. The results were nearly the same as those obtained from the single objective function minimizing nitrogen consumption baseline scenario (OF2). This indicates the objective function of minimizing nitrogen con-



sumption dominates in terms of directing results, perhaps because it aligns more with the dietary constraints which need to be satisfied. The rationale behind this conclusion goes back to the premise that NUE considerations focus on the plant and livestock scale and related processes. On the other hand, nitrogen consumption is more holistic in that it covers total nitrogen consumption (both natural and added) and accounts for the magnitude of the resulting quantity which directly plays into other WEF nexus components such as water and energy required for additional fertilizer production in addition to environmental impacts that are constrained by the planetary boundary.

0.5

0.8

Self Sufficiency Ratio

5. Conclusion

0.44

20

Nitrogen Consumption (kgN/capita/yr)

We present an optimization model that aids decision makers to make nitrogen-efficient choices while accounting for water, energy, and food security targets. The model is multi-scale, rendering it flexible for applications across multiple spatial and temporal levels. The model can be applied on a farm level targeting crop cultivation or on a higher (national or regional) level accounting for imports and exports. In addition, food consumption is accounted for daily representing a fine temporal scale, whereas production and trade values are determined aggregately over a yearly basis. Aside from crops and food, the model incorporates multiple water and energy resources with the appropriate processing/treatment technologies. These resource considerations are subject to nutritional constraints that ensure a minimal/maximal intake of required nutrients. As such, the model showcases the interactions between nitrogen and other WEFN actors and demonstrates the role of nitrogen in overall food security. To the authors knowledge, this work is the first of its kind, presenting a nitrogen focused optimization model that can be used to drive food security, while accounting for WEFN interlinkages and considerations.

A generic case study is developed to validate the model and illustrate the dependence of nitrogen variables on available natural resources, as well as dependence of food security on nitrogen. Case study results indicate that maximizing system nitrogen use efficiency results in the selection of crops with high N removal rates but does not account for actual nitrogen input requirements, thus potentially costing the system a relatively higher per capita N consumption rate, and high N losses. On the other hand, minimizing nitrogen consumption favors organic and recycled nitrogen sources and plant-based diets. Thus, this work emphasizes

1

the importance of accounting for both nitrogen consumption and nitrogen use efficiency considerations when setting policy targets, as a high NUE does not ensure a low nitrogen input and vice versa. A significant difference between the application of the two objectives (minimizing nitrogen consumption versus maximizing nitrogen efficiency) is the amount of resources needed to achieve the objective, where maximizing nitrogen efficiency was found to require more water and land. Here, it is necessary to acknowledge that those results come from a generic case study created for validating the operation of this model, and thus should be treated that way. We understand that each region will have its owns specificities, and hope that the results presented in this study can guide and inspire modelers and policy makers on directions to follow and questions to ask as they model their own specific regions.

Beyond nitrogen management, the study reveals how WEF nexus dynamics are significantly impacted by nitrogen. The change in food diet resulting from varying water and cropland availability validates the interdependence of WEFN components, and thereby reinforces the importance of holistic and integrated assessments that ensure improvement in one WEFN area does not come at the expense of another. Accounting for such interdependencies, particularly as relates to water, energy, or food securities, provides decision makers with more comprehensive assessments for more informed decision making.

It is important to acknowledge the model limitations, particularly that this model addresses the nitrogen problem from the supply side as opposed to the losses side. It focuses on minimizing nitrogen input and maximizing crop nitrogen removal, given the available resources and technologies. Future improvements can assess nitrogen losses more thoroughly. The model also considers biological nitrogen fixation and synthetic fertilizer to be equal nitrogen input contributors, which may not be an accurate reflection of realistic contexts. Such distinctions can be broken down for more detailed assessment of nitrogen flows within the system.

However, such detail comes at the expense of high data dependency. In its present form, the nature of the model and the WEFN interlinkages it accounts for renders it a data intensive application. WEFN data, in general, is lacking in the literature and future applications of the model would require case study specific data that may be difficult to acquire (Khan et al., 2022). Delving into more detail, particularly at more nuanced scale of nitrogen flow can complicate the problem.

Furthermore, it is acknowledged that technologies, best management practices, and policy implications play a significant role in the nitrogen problem. Expanding the model to include additional factors such as effect of soil characteristics, climatic conditions, specific types of synthetic fertilizers/manure applications, and crop yield responses at a more detailed level would add to model effectiveness and accuracy. Accounting for cropping seasons and crop rotations is also important, as both play a highly significant role in nitrogen management practices. However, such additions would also increase model complexity and require an extensive amount of data that may not be readily available.

In addition to nitrogen considerations, the model can also be improved by advancing to a multi-objective optimization context that simultaneously accounts for all WEFN sectors (water, energy, and food sectors) in addition to nitrogen. This will expand the model to evaluate the nexus directly while simultaneously assessing nitrogen in WEF nexus interactions. Moreover, directly incorporating the time factor would allow for more realistic simulation of nexus applications while taking the economic aspect into account.

Nonetheless, this work provides a holistic assessment of nitrogen in the WEF nexus. It validates how food is affected by nitrogen constraints and how resource availability affects food. The correlation between food self-sufficiency and nitrogen consumption demonstrates the significance of applying the nitrogen planetary boundary constraint and sheds light on the role of trade in nitrogen flow dynamics. The model can serve as a decision support tool for policymakers by providing information that demonstrates how policy implications related to trade and resource management can affect food security, specifically, and resource security, overall.

Declaration of Competing Interests

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

All data used is summarized in the Supplement Materials.

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Supplementary materials

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