Refining a simplified nitrogen leaching method in grey water footprint assessment: a maize case study

Fig. 1: Nitrogen fertilizer application (Target-Fertilisers, 2022)

Master thesis

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Refining a simplified nitrogen leaching method in grey water footprint assessment: a maize case study

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Preface

This thesis marks the completion of my Master's in Civil Engineering and Management at the University of Twente. Over the course of this research, I have explored the optimization of a simplified model for calculating nitrogen leaching in agriculture. This process has deepened my understanding of nitrogen dynamics and the environmental impact of leaching during crop growth. Additionally, working on this project has significantly improved my programming and academic writing skills.

I would like to thank my supervisors, Maarten Krol, Han Su, and Oleksandr Mialyk for their guidance and support throughout this project. Their encouragement to think critically, refine my academic writing, and structure my methodology and results has been important in shaping this thesis. The insightful discussions and constructive feedback provided me with new perspectives and helped me develop a more systematic approach to my research.

Finally, I want to thank my family and friends for their support and for providing much-needed distractions during the past months.

Arjen Scholten
March 2025

Summary

This thesis addresses the critical challenge of nitrogen leaching from agricultural activities, which poses both economic and environmental risks. While some nitrogen loss to leaching is unavoidable, excessive nitrogen application has pushed total leaching levels beyond what ecosystems can tolerate, leading to groundwater contamination. In many cases, fertilizer is applied at rates that exceed not only environmental limits but also economic efficiency, where additional nitrogen no longer translates into higher yields. This imbalance between input and benefit highlights the need for more precise nitrogen management strategies. A key part of improving nitrogen management is the ability to accurately estimate leaching losses, allowing for better decision-making in fertilizer application.

To achieve this, accurate and practical methods for estimating nitrogen leaching, particularly in the context of grey water footprint calculations, are required. Three commonly used approaches are the Tier 1, 2 and 3 method. The Tier 1 method is a simplified approach that relies on generalized assumptions or a fixed leaching fraction, making it easy to apply but often lacking accuracy across different agricultural conditions. In contrast, Tier 2 and 3 are advanced modeling approach that incorporates detailed, region-specific data, providing more accurate estimates. However, its complexity and high data requirements limit widespread adoption. Since Tier 1 lacks the accuracy, but Tier 2 is often too data-intensive for practical use, this study focuses on evaluating and refining the Tier 1 method to improve its accuracy while maintaining its accessibility, narrowing the gap between simplicity and precision in nitrogen leaching estimation.

First, a Python-based automated script was developed to support the application of the Tier 1 method by both implementing the approach and automating the data input from global datasets, improving scalability and efficiency. Next, a literature review of Tier 2 and Tier 3 studies was conducted to compare their approaches with Tier 1 and identify key differences in nitrogen leaching estimation. A sensitivity analysis was then performed on the Tier 1 method to determine its most influential

parameters. Finally, based on these insights, key parameters were optimized to improve accuracy while maintaining the Tier 1 method's simplicity.

While automation successfully integrated datasets such as nitrogen application rates, soil texture, and precipitation, certain inputs such as soil texture, drainage class and management practices still required manual entry due to the lack of a suitable global datasets. Despite this, the automated Tier 1 method demonstrated high accuracy compared to other Tier 1 studies, with minimal bias and low variance in its results, making it a reliable tool for Tier 1 calculations in this thesis.

The study identified the most influential factors in the Tier 1 method and took insights from the Tier 2 and 3 method. From this analysis the nitrogen application rate emerged as the most practical factor for optimization due to its high data availability and significant impact on leaching outcomes. Optimization efforts focused on adjusting the weight of nitrogen application rates and increasing the maximum leaching fraction (α_{max}) in the Tier 1 equation. By raising α_{max} from 0.25 to 0.475 and increasing the application rate weight to 20%, the refined Tier 1 method reduced RMSE and MAE by more than 20%, aligning more closely with Tier 2 results. While the original Tier 1 method has a systematic negative bias, underestimating leaching, the optimized version has a slight positive bias, improving alignment with observed field values on average but still struggling to accurately predict individual data points.

In conclusion, this thesis demonstrates that the Tier 1 method can be effectively refined to improve its accuracy while maintaining its simplicity and scalability. The refined and automated Tier 1 method developed in this study provides a more user-friendly and accurate tool for assessing nitrogen leaching than the original Tier 1 method of Franke et al. (2013), but its ability to support sustainable nitrogen management remains limited by its inability to capture results from advanced models or field experiments.

Future research should expand the literature review to improve dataset variability, ensuring better representation of key factors. Conducting an early multi factor exploratory analysis would help identify dataset gaps and refine nitrogen application influences. Further improvements should focus on automating soil texture and drainage classification, quantifying management practices, and integrating higher-resolution datasets for nitrogen fixation, plant uptake, and application rates.

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1 Introduction

Agriculture relies heavily on fertilizers to improve crop growth and health, with nitrogen being the primary source (Alnaass et al., 2024). In the soil, there is often sufficient total nitrogen, but not enough plant-available nitrogen (such as nitrate or ammonium) to optimally supply the crop (Robertson et al., 2009). To address this nitrogen gap, farmers worldwide use fertilizers, applying either organic sources like manure or synthetic alternatives. Over the past decades, the global mean nitrogen fertilizer application rate has steadily increased. In 1990, the average application rate was approximately 50 kgN per hectare of cropland, rising to 70 kgN per hectare by 2020, before declining slightly to 65 kgN/ha in 2022 (FAOSTAT, 2024a). However, there are considerable regional variations in nitrogen application rates, influenced by factors such as soil fertility, economic constraints, agricultural practices and policy interventions. In North America and Europe, rates range between 60–100 kgN/ha and have begun to level off, while in Asia rates are notably higher and continue to rise, reaching 110–230 kgN/ha. In contrast, many countries in Sub-Saharan Africa apply significantly lower amounts, often as little as 10 kgN/ha, often due to economic constraints and limited access to fertilizers (World-data, 2024).

The increase in nitrogen fertilizer application has been important for boosting crop yields to meet the crop demands of a growing global population. Although plants absorb a substantial portion of the nitrogen, a significant amount often remains unused due to excessive or inefficient use of nitrogen fertilizers, leading to environmental issues such as water pollution, greenhouse gas emissions, and soil degradation. This inefficiency is driven by several factors such as excessive application, poor timing, or unfavourable weather conditions (EOS, 2024). Traditionally, farmers have applied more fertilizer than crops require to maximize yield and profitability. However, this approach is increasingly recognized as unsustainable (Kitchen et al., 2008). The unused nitrogen can leach through the soil as water moves downwards, especially in sandy or coarse-textured soils where water drains quickly. Leaching is also more likely to occur during periods of excessive precipitation or irrigation, which saturates the soil and pushes water and the dissolved nitrogen beyond the crop's root zone (ESN, 2024). Therefore, adopting sustainable nitrogen management practices is crucial to balance agricultural productivity with environmental conservation.

The loss of nitrogen through leaching is a major concern in agriculture because it represents both an economic loss for farmers and an environmental hazard. For farmers, leaching represents waste of a valuable and costly resource. Nitrogen fertilizers are expensive, and when they leach away, farmers lose a portion of their investment in crop productivity. This can lead to reduced yields if insufficient nitrogen remains available for plant uptake, forcing farmers to apply additional fertilizer, further increasing their costs. More significantly, nitrogen leaching poses serious environmental and public health risks. Nitrogen that leaches into groundwater can contaminate drinking water supplies, and it can also enter rivers, lakes, and coastal waters through runoff (Hina, 2024).

Determining the leaching of excessive nitrogen application presents several challenges. Firstly, numerous factors influence nitrogen leaching, including climate conditions, soil type, texture, land characteristics, management practices, and field drainage patterns (Rupp et al., 2024; Bibi et al., 2016). Secondly, while field experiments offer precision, they demand substantial investments in both time and money. Additionally, their small-scale nature and the unique factors of each field make extrapolating results difficult. This is where modelling becomes important, offering relatively accurate results in a faster and more cost-effective way by making certain assumptions. Although modelling results may be an approximate value and not the exact value, they still reveal large-scale patterns and can incentivize farmers to adopt environmentally friendly practices (Mandrini et al., 2022).

1.1 Three-tier approach in Water Footprint Assessment

The water footprint assessment (Hoekstra et al., 2012) categorizes water use into three components: green, blue and grey water footprints. The green water footprint relates to the volume of precipitation consumed (evapotranspired) by a crop during the entire growth process. The blue water footprint involves the consumptive use of surface and groundwater resources withdrawn for irrigation that are not returned to their source. The grey water footprint measures the amount of freshwater required to dilute pollutants, such as nitrogen, to meet acceptable water quality standards (Hoekstra et al., 2012). Accurate calculation of the grey water footprint depends on precise estimation of the pollutant levels. To assess how much nitrogen leaches and runs off during crop growth, a three-tier approach was developed by the Water Footprint Network (Hoekstra et al., 2011). Advancing from Tier 1 to Tier 3, the accuracy of estimation improves, but the feasibility and scalability of the analysis decrease because higher tiers require more detailed data, making it more challenging to repeat the method across different regions, crops, or systems without excessive data and resource demands.

Tier 1 can be seen as the most simplistic, where a fixed fraction or a rough calculation is used to estimate the amount of chemical leaching to the groundwater or surface water system. Tier 2 involves a more data-intensive process, using standardized or simplified models based on data such as management practices, local soil attributes, and climatic conditions. Tier 3 is the most advanced way of estimation and uses process-based modelling techniques and may require on-site measurements. It provides the most accurate and reliable results but requires substantial resources and is challenging to implement widely.

1.1.1 Tier 1

Within Tier 1, the nitrogen leaching-runoff fraction can be calculated using four distinct methods, each using one of two underlying approaches. The first approach involves determining the leaching-runoff fraction (α) of the entire nitrogen applied to estimate the total nitrogen leaching. Alternatively, the second approach calculates the nitrogen surplus, defined as the total nitrogen applied minus the crop offtake. This leaching-runoff fraction (β) is higher than in the first approach due to the higher boundaries, as shown in Table 1.2. While under reasonable N-application rates, the results of both approaches can yield similar results, they deviate at excessive rates. when the soil reaches saturation, the surplus in nitrogen increases which leads to greater nitrogen leaching in the second approach.

Table 1.1 presents an overview of the four Tier 1 methods, arranged from least to most preferable and from least to most data demanding. Methods 1 and 2 are simpler to execute, whereas methods 3 and 4 offer greater accuracy although with increased complexity. The nitrogen surplus methods are favoured due to the significant variability in crop offtake across different crop types (Franke et al., 2013).

Tab. 1.1: Overview of the Tier 1 methods for estimating the nitrogen leaching-runoff fraction

	Method
1.	Assumed or average leaching-runoff fraction (α) times nitrogen application
2.	Assumed or average leaching-runoff fraction (β) times nitrogen surplus
3.	Estimated leaching-runoff fraction (α) (calculated with leaching-runoff potential) times nitrogen application
4.	Estimated leaching-runoff fraction (β) (calculated with leaching-runoff potential) times nitrogen surplus

1.1.1.1 Assumed leaching-runoff fraction

As shown in Table 1.1 the Tier 1 methods are divided into a simple (method 1 & 2) and somewhat more extensive methods (method 3 & 4). The simpler options involve using an assumed or average leaching-runoff fraction, facilitating a quick and straightforward analysis suitable for exploring large-scale patterns. However, this approach lacks precision as it overlooks crucial local factors such as soil characteristics, climatic conditions, and agricultural practices, which can significantly influence the leaching-runoff fraction (Franke et al., 2013).

Despite their limitations, these methods are widely used in global studies or as an initial assessment in water footprint. Studies such as those conducted by Gobin et al. (2017), Mekonnen et al. (2014), and Yin et al. (2022) have used the average leaching-runoff fraction (α) of 10%. However, Mekonnen et al. (2015) used a higher α value of 18%.

1.1.1.2 Estimated leaching-runoff fraction

The somewhat more extensive methods involve estimating the leaching-runoff fraction based on several local variables with the help of the following two equations: 1.1 (for method 3) and 1.2 (for method 4).

The equation for α calculates the leaching-runoff fraction assuming a linear dependency on each of the factors considered. Eventually, the grey water footprint can be calculated with the α and the nitrogen application rate. The equation adjusts the value of α within the specified range of α_{min} to α_{max} using a weighted average of several factors:

$$\alpha = \alpha_{\text{min}} + \left[\frac{\sum_i s_i \cdot w_i}{\sum_i w_i} \right] \cdot (\alpha_{\text{max}} - \alpha_{\text{min}}) \tag{1.1}$$

Where:

- α_{min} and α_{max}: Represent the minimum and maximum possible leaching-runoff fractions for the application-based method, from Table 1.2.
- s_i: The score assigned to each factor, ranging from 0 to 1, where 0 relates to a very low leaching potential and 1 for the highest possible leaching potential.
- w_i: The weight of each factor, from Figure 5.1 in the appendix.
- $\frac{\sum_i s_i \cdot w_i}{\sum_i w_i}$: Represents the weighted sum of the scores (s_i) for each factor, divided by the total weight (w_i). This accounts for the relative contribution of each factor based on its assigned weight.

By adding this weighted term to α_{min}, the equation ensures that the resulting α lies within the specified range and accounts for the cumulative influence of all contributing factors.

Similarly, the equation for β (Equation 1.2) calculates the leaching-runoff fraction based on the nitrogen surplus method, unlike Equation 1.1, β operates over a wider range and calculates the grey water footprint using the nitrogen surplus rather than the application rate. The nitrogen surplus accounts for the nitrogen applied minus the nitrogen offtake, which is the amount of nitrogen absorbed by the crop and harvested.

$$\beta = \beta_{\text{min}} + \left[\frac{\sum_i s_i \cdot w_i}{\sum_i w_i} \right] \cdot (\beta_{\text{max}} - \beta_{\text{min}}) \tag{1.2}$$

Where:

- β_{min} and β_{max}: Represent the minimum and maximum possible leaching-runoff fractions for the surplus-based method.
- The other parameters (s_i, w_i, and the weighted average) are defined similarly to those in Equation 1.1.

According to Franke et al. (2013), these equations bound the resulting values within minimum and maximum thresholds (Table 1.2), which they consider to represent realistic leaching-runoff scenarios.

Tab. 1.2: minimum, average, and maximum values for leaching-runoff fractions for both the application-based (α) and surplus-based (β) method.

	Application-method		Surplus-method	
Minimum leaching-runoff fraction	α_{min}	0.01	β_{min}	0.08
Average leaching-runoff fraction	α_{avg}	0.1	β_{avg}	0.44
Maximum leaching-runoff fraction	α_{max}	0.25	β_{max}	0.8

Both equations compute values (α and β) that represent the leaching-runoff fraction for nitrogen, both equations are based on specific local variables, such as:

- Atmospheric deposition: Nitrogen from the atmosphere deposits onto land surfaces. This has a significant impact, as higher deposition rates mean a more saturated retention capacity of the soil, increasing the likelihood of leaching.
- Soil texture: This refers to the composition of soil particles, which can vary widely and impact the soil's ability to retain water and nutrients. Soil with larger particles, like sand, has larger pore spaces between particles, allowing

water to move more freely. However, this also means that water drains more quickly through sandy soil, carrying nutrients like nitrogen with it.

- Natural drainage patterns: This refers to how water moves through the soil, which can vary each field. Poorly drained soils may have low leaching rates but are prone to runoff losses after heavy rain.
- Climate conditions: Particularly precipitation patterns can cause a sudden peak in leaching, especially after a dry period. When the retention capacity of the soil is exceeded, the nitrogen is transported quickly through the soil profile or is lost through overland flow.
- Agricultural management practices, including the timing and method of nitrogen application, irrigation practices, and tillage methods, can greatly affect nitrogen dynamics in soils. Excessive irrigation, for example, can increase soil water content and facilitate leaching. Implementing best management practices tailored to specific crops and local conditions is crucial for optimizing nitrogen use efficiency.

While the estimation methods may be time-consuming, especially in global studies, they offer a feasible and scalable solution for local assessments on various scales, including national, provincial, or on farm level if the appropriate data is available, as shown by Gil et al. (2017), and Muratoglu (2020).

1.1.2 Tier 2 and Tier 3

In contrast to the generalized assumptions or fixed leaching fractions used by Tier 1, Tier 2 and Tier 3 methods rely on more detailed modeling approaches, incorporating site-specific variables to improve accuracy. Tier 2 methods typically use models that simulate agricultural and environmental processes based on available regional or site-specific data, striking a balance between complexity and practicality. In contrast, Tier 3 methods employ fully process-based modeling approaches combined with extensive field studies and direct site-measurements, providing the most accurate nitrogen leaching estimates but requiring substantial data inputs.

Several widely used models fall within these categories, differing in scope and complexity. At the field scale, Tier 2 models such as DSSAT (Decision Support System for Agrotechnology Transfer) simulate crop growth, soil interactions, and management effects (Jones et al., 2003), while EPIC (Environmental Policy Integrated Climate) integrates soil, weather, crop growth, and management practices to assess the environmental and economic impacts of nitrogen use (Lychuk et al., 2021). At a larger spatial scale, the SWAT (Soil and Water Assessment Tool) model evaluates nitrogen transport across landscapes by incorporating land use, hydrology, and management practices (Akhavan et al., 2010).

In contrast, Tier 3 models, which rely on fully process-based simulations and extensive field data, include HYDRUS-2D, which models water, nutrient, and solute movement in unsaturated soils, making it particularly useful for studying leaching dynamics (Šimůnek et al., 2016). RZWQM(2) (Root Zone Water Quality Model) evaluates how different agricultural practices affect water and nitrogen movement within the root zone (Hanson et al., 1998). APEX (Agricultural Policy/Environmental eXtender), while often applied at a watershed scale, incorporates detailed process-based simulations, aligning it with Tier 3 methodologies (Chukalla et al., 2018).

While these models vary in complexity and scale, they provide valuable insights for refining Tier 1 nitrogen leaching estimates. Additionally, this study incorporates field experiments, which are considered part of Tier 3, as they provide direct measurements of nitrogen leaching under different conditions. However, the distinction between Tier 2 and Tier 3 models is not essential for this research, as both are used to evaluate and improve the Tier 1 approach.

1.2 Problem Statement

Nitrogen fertilizers play a critical role in supporting global food production by promoting plant growth and improving agricultural productivity. However, the inefficient and excessive application of nitrogen fertilizers leads to significant nitrogen leaching, particularly in coarse-textured soils or under excessive precipitation and irrigation conditions. This leaching not only represents an economic loss for farmers but also poses severe environmental and public health risks (Hina, 2024; Dybowski et al., 2020).

While detailed field experiments can accurately measure nitrogen leaching, they are often costly, time-consuming, and challenging to scale due to variations in climate, soil properties, and management practices. As a result, water footprint assessments rely on estimation methods that balance accuracy, feasibility, and scalability. The Tier 1 approach, which uses assumed or estimated leaching-runoff fractions, is widely adopted for its simplicity and lower data requirements. However, it lacks the precision of the more advanced Tier 2 approach, which incorporates site-specific variables and environmental models to improve accuracy.

This creates a gap: the Tier 1 method is practical and accessible but imprecise, while the Tier 2 method is more accurate but complex and data-intensive. The inability of Tier 1 to reliably estimate nitrogen leaching undermines its utility for sustainable nitrogen management and water footprint assessments. Narrowing this gap is essential to provide farmers, policymakers, and researchers with a tool that balances usability, accuracy, and scalability.

Conducting a Tier 1 study involves significant manual effort, as researchers must identify, extract, and process data from various sources. This approach is time-consuming and prone to errors, particularly when dealing with the large datasets required for accurate nitrogen leaching-runoff calculations. Furthermore, finding relevant, location-specific data for each study can be a complex and inefficient task when done manually.

Automating this process with a Python script improves efficiency, consistency, and scalability. By integrating predefined links to global datasets, automation allows for the quick retrieval of necessary environmental variables, reducing the time and effort required to locate and process data. Additionally, by minimizing human input errors, automation ensures that nitrogen leaching estimates are more reliable and reproducible. These improvements are essential for making Tier 1 studies more practical and scalable across different locations and agricultural systems.

To analyze and refine the Tier 1 method, this study focuses on maize, the most widely produced cereal crop globally, playing a crucial role in global food security and livestock feed production (FAOSTAT, 2025). It has become one of the most nitrogen-intensive crops (Adalibieke et al., 2023; Heffer et al., 2016). This makes maize a particularly relevant crop for studying nitrogen leaching dynamics.

The first step in addressing this problem is to evaluate the accuracy of the Tier 1 method and identify potential refinements that could improve its performance. This study systematically optimizes key parameters, including α_{max}, which sets the upper limit of the leaching fraction, and the weight of the N-application rate, which is a key contributor to nitrogen leaching and has significantly higher data availability to other factors. By doing so, it investigates whether Tier 1 can achieve accuracy levels closer to Tier 2 while maintaining its simplicity. If successful, it could enable better nitrogen management practices, reduce environmental impacts, and support sustainable agriculture on local and global scales.

1.3 Research objective

The objective of this thesis is to evaluate and refine the current Tier 1 nitrogen leaching-runoff approach to better match the results from the more detailed Tier 2 and 3 approaches while retaining the key advantages of the Tier 1 approach. These advantages include its lower data requirements, which reduce complexity, and its ease of use, making it accessible and practical for broader regional and global applications.

1.4 Research questions

In order to fulfil the research objective, three research questions were formulated.

1. How does the performance of the Tier 1 estimation method compare to Tier 2 and 3 in estimating the nitrogen leaching fraction?
2. Which factors in the Tier 1 estimation method are most significant in determining the leaching-runoff potential?
3. How can the Tier 1 nitrogen leaching estimation method be optimized to better align its results with Tier 2 and 3 studies?

2 Methodology

Refining the current Tier 1 estimation method requires a structured research approach, as illustrated in the flowchart in Figure 2.1. The process begins with the automation of the Tier 1 estimation method through the development of a Python script that streamlines the calculations, reducing manual effort and integrating global datasets. Next, a literature review is conducted to evaluate the performance of the Tier 1 method compared to Tier 2 and field studies, identifying deviations and potential refinements. A sensitivity analysis follows to determine the most influential factors within the Tier 1 method. Subsequently, a parameter optimization process is carried out using a subset of the literature review data. Finally, the optimized model is validated against the remaining dataset to ensure its performance remains reliable beyond the calibration dataset.

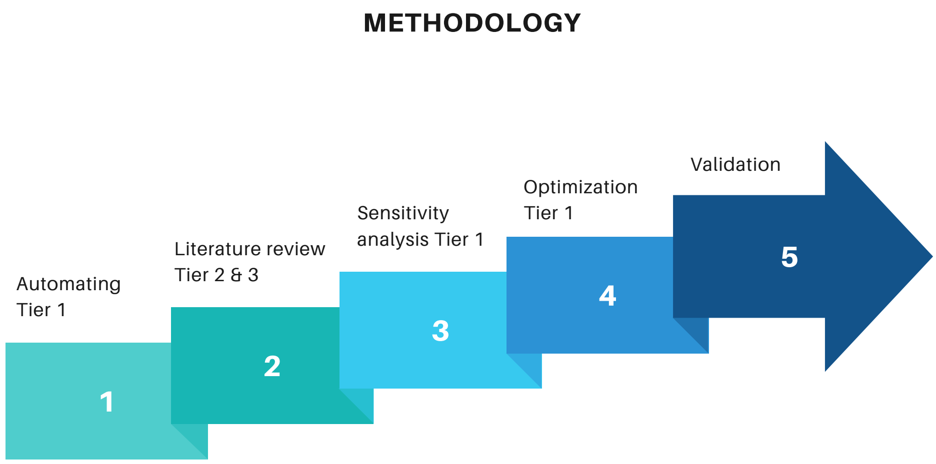


Fig. 2.1: Research methodology flowchart

2.1 Tier 1 python program

This section outlines the systematic approach used for automating the Tier 1 estimation method. A Python script was developed to identify, extract, and process data from multiple global datasets, reducing the need for manual effort. The script integrates predefined links to these datasets, enabling the retrieval of location-specific information based on geographic coordinates or other inputs. By automating this workflow, the script ensures a more efficient and consistent approach to the Tier 1 method.

The Tier 1 estimation methods is based on Equation 1.1 and Equation 1.2, which calculate the nitrogen leaching-runoff fraction by incorporating multiple environmental and agricultural factors, such as:

- Atmospheric nitrogen deposition
- Soil texture
- Soil drainage class
- Precipitation
- Nitrogen fixation
- Nitrogen application rate
- Plant uptake
- Management practice

To start of the process appropriate worldwide datasets are identified for all the factors. To gather relevant datasets, an extensive review of online databases and environmental portals, such as the Food and Agriculture Organization (FAO), NASA, and the World Bank, was conducted. Evaluation criteria were established to ensure the selected datasets were suitable for use. These criteria included the use of a compatible unit commonly used in other nitrogen leaching studies, which is kgN/ha/year for the nitrogen application rate. Both temporal and spatial resolution were considered, ensuring that factors such as nitrogen deposition and precipitation were available at appropriate intervals and spatial scales, making them suitable for broad regional studies. However, the selection of datasets was constrained by both data availability and computational efficiency. While higher-resolution datasets exist for some variables, they often come with significantly longer processing times, making them impractical for large-scale applications. Lastly, it was essential that the data was formatted in a file type compatible with python. The datasets selected for the script are listed in Table 2.1. However, the datasets for soil type and drainage class were not suitable for automation, and no dataset was available for management practices. As a result, three out of the eight factors could not be automated and require manual input, which will be explained later. Once the relevant datasets were identified, the next phase involved developing and testing the Python script to retrieve and process this data.

Tab. 2.1: Overview of factors, their corresponding spatial and temporal resolution, unit, and data sources.

Factor	Spatial res.	Temporal res.	Unit	Source
N-deposition	56 x 56 km	Annual	KgN/ha	(ISIMIP, 2024)
Soil type	1 x 1 km	-	-	(HWSD, 2024)
Drainage class	1 x 1 km	-	-	
Precipitation	278 x 278 km	Monthly	Mm	(GPCP, 2024)
N-fixation	Country	Annual	KgN/ha	(FAOSTAT, 2024b)
Plant uptake	Country	Annual	KgN/ha	
Application rate	Country	Annual	KgN/ha	(Ludemann et al., 2022)
Management practices	Country	-	-	-

To begin using the script for a specific case study, a set of essential inputs is required to ensure that the calculations for the nitrogen leaching-runoff fractions are accurate, an example is shown in Table 2.2. One of the primary inputs needed is the country name and the crop type, which are used to retrieve N-fixation, plant uptake data and the appropriate nitrogen application rate from their dataset. The information for each factor is sourced from a CSV file that contains country and crop-specific application rates for several years, enabling the script to match the provided input with the correct values for use in the calculation. In some cases, deviations arise between country names used in the different datasets due to variations in naming or differences in regional definitions. This is particularly relevant when aligning application rate data with N-fixation or plant uptake datasets. For example, some dataset may use "China" while the others specify "China, mainland" or one may use "Turkey" while the other uses "Türkiye". When this occurs, the script allows for an alternative country name (country2) to be used for the N-fixation and plant uptake datasets, ensuring consistency and accurate data matching.

Tab. 2.2: Example of input variables for the automation script.

Input variables	Manual input values	Used for which dataset
Country	China	App. rate
Country2	China, mainland	N-fix. and plant uptake
Crop	Maize	App. rate, N-fix. and plant uptake
Longitude	38.9333	N-dep. and precipitation
Latitude	115.5333	N-dep. and precipitation
Management practices	Worst	-
Soil type	7	-
Drainage class	P	-

For other environmental factors, geographical coordinates (longitude and latitude) must be provided to pinpoint the location for which the leaching-runoff fraction is being calculated. These coordinates are crucial for extracting location-specific data such as N-deposition and precipitation from the respective datasets. The N-deposition data is sourced from a NetCDF (.nc4) file, which the script can directly access once the coordinates are provided. Similarly, precipitation data is obtained from a .nc file.

The soil type and drainage class were not automated yet and still require manual input due to the absence of a suitable dataset for the drainage classes. While automating soil type seperately might have been possible, the viewer displays both soil type and drainage class together. Therefore, searching for a better soil type dataset was unnecessary, as the drainage class remained the limiting factor. These factors can be identified using the HWSD2 viewer, which is a global soil database that provides detailed information on soil characteristics. To obtain this data, the user has to pinpoint at the same coordinates as previously used for other factors in the HWSD2 viewer, and manually search for the corresponding soil type and drainage class, and then transfer this information into the script. The identified soil type is selected from a list of 13 possible categories, ranging from heavy clay to sand, each of which plays a critical role in influencing the nitrogen leaching potential of the soil. The drainage class, similarly, has seven possible categories, from "Very poorly drained" (VP) to "Excessively drained" (E), which also significantly affects the potential for nitrogen runoff. The soil texture and drainage class inputs are shown in Table 5.1 in the appendix.

The script also requires input regarding management practices. In the original methodology, this involved a detailed yes/no questionnaire, which was often too specific for broader studies that cover larger regions. To simplify this process, the script allows users to input a general assessment of management practices as "best," "good," "average," or "worst." This simplification makes it easier to estimate management efficiency.

2.2 Tier 2 and 3 analysis

To address the first research question, “How does the performance of the Tier 1 estimation method compare to Tier 2 and 3 in estimating the nitrogen leaching fraction?”, an extensive literature review was conducted, that focuses on Tier 2 and Tier 3 (field) studies. An initial search, with the following description: ("leaching rate" OR "leaching loss" OR "leaching fraction" OR "leaching ratio") + "maize" yielded 110 research papers, from which 25 studies were selected that reported nitrogen leaching results for one or a few cases.

For a study to be deemed appropriate for this analysis, it needed to specify essential variables: the location of the research site, the nitrogen application rate, and the nitrogen loss in kilograms per hectare (kg/ha). These criteria ensured that the data was both relevant and comparable across studies. Among the selected papers, 11 out of those 25 were Tier 2/3 studies, and 14 were field experiments. Figure 2.2 highlights the geographical distribution of studies from the literature review.

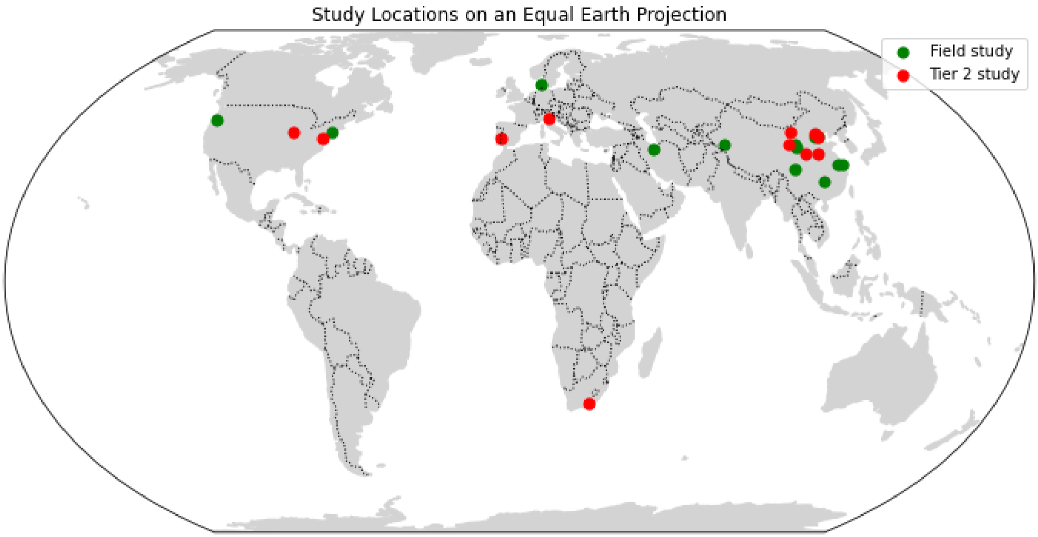


Fig. 2.2: Geographic distribution of study locations identified from the literature review, representing field experiments and Tier 2/3 studies across multiple countries.

The more specific characteristics, such as the soil texture and number of observations of each study are shown in Table 2.3. Most studies are a multi-year investigation between two and five years providing insights into temporal variability and soil behaviour. Additionally, many studies test different methods in applying fertilizer or management practices such as irrigation techniques, crop covering, and reducing tillage. All studies are based on maize or a rotation between maize and soybeans.

Once relevant Tier 2 and field studies are identified, the next step is to apply the Tier 1 estimation method to the same case studies from the literature review. This

Tab. 2.3: Summary of study locations obtained from the literature review, including country, study/model type, soil texture, number of observations (Obs.), and references for each study.

Country	Region	Type	Soil texture	Obs.	Reference
USA	Illnois	APSIM	Silty loam	6	(Pasley et al., 2021)
USA	Arlington	IBIS	Silty loam	3	(Kucharik et al., 2003)
China	Xianyang	RZWQM2	Silty loam	5	(Xu, Cai, et al., 2020)
China	Tianjin	WHCNS	Silt	8	(Liang et al., 2020)
China	Qiaodi	RZWQM2	Silty loam	5	(Xu, Wang, et al., 2020)
China	Bayannaoer	APSIM	Sandy loam	3	(Ren et al., 2024)
China	Yuzhou	RZWQM2	Sandy loam	1	(Ding et al., 2020)
Italy	Po Valley	SWAP	Loamy clay	5	(Perego et al., 2012)
China	Changping	DNDC	Silty loam	3	(Y. Zhang et al., 2015)
Spain	Badajoz	APEX	Loam	7	(Chukalla et al., 2018)
South-Africa	Nxuba	EPIC	Sandy clay loam	10	(Choruma et al., 2021)
China	Tongxin	Field	Loam	6	(Guo et al., 2023)
China	Qiyang	Field	Sandy loam	3	(Huang et al., 2017)
USA	New York	Field	Silty loam	17	(Sogbedji et al., 2000)
China	Ya'an	Field	Sandy clay loam	8	(Yao et al., 2021)
China	Xushui	Field	Sandy loam	4	(Du et al., 2019)
USA	Corvallis	Field	Sandy loam	4	(Weitzman et al., 2022)
China	Yutian	Field	Clay	8	(Fan et al., 2017)
China	Tianjin	Field	Clay loam	5	(J. Zhang, He, et al., 2020)
Iran	Tehran	Field	Sandy loam	24	(Gholamhoseini et al., 2013)
China	Yixing	Field	Loamy clay	6	(Qiao et al., 2022)
China	Qingpu	Field	Silty loam	12	(J. Zhang, Sha, et al., 2015)
China	Pengyang	Field	Sandy loam	20	(Liu et al., 2023)
Iran	Tehran	Field	Sandy loam	6	(Gholamhoseini et al., 2013)
Denmark	-	Field	Sand	6	(Simmelsgaard, 2007)

step involved gathering the necessary input data for the Tier 1 calculation, using the same geographic regions and conditions as the Tier 2 studies. In cases where the Tier 1 method is already included in the Tier 2 study, the existing data will be utilized for direct comparison. If not, the Tier 1 method will be independently applied using global datasets to replicate the conditions as accurately as possible. This can possibly lead to minor deviations in the results due to the use of different datasets compared to those used in the Tier 2 study, which are often more detailed and specific to the area of interest.

2.3 Identifying key factors in Tier 1

To address the second research question, “Which factors in the Tier 1 estimation method are most significant in determining the leaching-runoff potential?”, a case study was selected, and a sensitivity study was conducted. The objective was to evaluate the significance of each individual factor and their influence on the leaching-runoff fraction, and see if modifications to the equation would narrow the gap between Tier 2 and 1. The case study was conducted in South-Africa, based on the work of Choruma et al. (2021), because it was well-documented and used a broad range of N-application rates. The Tier 1 method was configured using the same nitrogen application rate and other relevant local input values used in the Tier 2 study. While this specific case study was used, it is expected that another case studies would yield comparable ranges for each factor. The focus of the sensitivity analysis is on the significance of the individual factors themselves, rather than the unique attributes of the selected case study.

To determine the influence of each factor, a sensitivity analysis was conducted, by manually modifying one factor at a time while keeping the others constant. This approach enabled the isolation of individual effects and facilitated the identification of the most impactful factors. For example in the original Tier 1 calculation for this case study the N-deposition is very low and assigned a value of 0. To test the equation the N-deposition is set at very high with a value of 1. The resulting changes in the leaching fraction were then compared and plotted to the Tier 2 study. This process was repeated for all factors to evaluate their relative impact on the Tier 1 method. While the primary objective of the sensitivity analysis was to examine how changes in individual factors affect the Tier 1 leaching estimates. The comparison with Tier 2 aimed to assess whether Tier 1 consistently underestimates leaching or if certain conditions allow it to produce similar estimates.

After the analysis of all the factors, the focus shifted to improving the accuracy of the equation with the help of two modifications: adjustment of the weight of the application rate, and increasing the α_{max}, which limits the predicted value of the Tier 1 method. The outcomes of the modified scenarios were compared to the results of the original Tier 1 calculations and the Tier 2 study, which served as the benchmark for the accuracy.

2.4 Tier 1 optimization

In the previous chapter only a single parameter in the equation was modified at the time, but this is ultimately insufficient to narrow the gap between the Tier 1 and Tier 2 approaches. To address this, an optimization process involving a combination of the previously explained modification was implemented. A Python script was developed specifically for this purpose. From the original literature review dataset, 15 studies were randomly selected for optimization, while the remaining studies were used for validation. Some control was applied in the selection process to ensure that both Tier 2 and field studies were represented in both the optimization and validation sets. These studies are listed in Table 2.4.

Tab. 2.4: Randomly picked studies from the literature review used for optimization.

Optimization studies					
Country	Region	Type	Soil texture	Obs.	Reference
China	Tianjin	WHCNS	Silt	8	(Liang et al., 2020)
Italy	Po Valley	SWAP	Loamy clay	5	(Perego et al., 2012)
China	Qiaodi	RZWQM2	Silty loam	5	(Xu, Wang, et al., 2020)
South-Africa	Nxuba	EPIC	Sandy clay loam	10	(Choruma et al., 2021)
USA	Arlington	IBIS	Silty loam	3	(Kucharik et al., 2003)
USA	Illinois	APSIM	Silty loam	6	(Pasley et al., 2021)
China	Yixing	Field	Loamy clay	6	(Qiao et al., 2022)
China	Pengyang	Field	Sandy loam	20	(Liu et al., 2023)
China	Tianjin	Field	Clay loam	5	(J. Zhang, He, et al., 2020)
USA	Corvallis	Field	Sandy loam	4	(Weitzman et al., 2022)
USA	New York	Field	Silty loam	17	(Sogbedji et al., 2000)
China	Qingpu	Field	Silty loam	12	(J. Zhang, Sha, et al., 2015)
China	Tongxin	Field	Loam	6	(Guo et al., 2023)
China	Yutian	Field	Clay	8	(Fan et al., 2017)
Iran	Tehran	Field	Sandy loam	24	(Gholamhoseini et al., 2013)

The optimization process focuses on two key parameters in the equation: α_{max} and the weight for the application rate. α_{max} serves as the backbone of the equation, significantly impacting the overall results, a higher α_{max} increases the calculated values substantially. The application rate is equally crucial, based on the literature study that was conducted, where field and model studies show a significant rise in leaching fraction when the application rate increases. So to make the application rate more influential in the equation, the weights will be alternated. When the weight of the application rate increases, another weight has to decrease. This decision is based on the results of section 3.3 which highlights the factors that are less influential in the equation. To make the optimization process easier, upfront ten weight sets are made with different weights for the application rate, increasing with steps of 5%, from the original 10% up to 55%. The maximum of 55% was used to ensure each of the other factor contributes at least 5%, preventing any factor from being entirely neglected. In the original Tier 1 method, the minimum weight was also 5%, but no clear justification was given for this choice or for the allocation of the other weights. The weight sets are shown in the appendix in Table 5.2.

To perform the optimization, the script uses the scipy.optimize.minimize library. A total of nine optimizations were conducted, each corresponding to a different weight set, treated as a discrete variable. In each case, α_{max} was optimized as a continuous variable, adjusting accordingly and taking any value within the range of 0.25 to 1.

To determine the best α_{max} and weight set, the RMSE (Root Mean Square Error) and MAE (Mean Absolute Error) were used. These are widely recognized metrics for evaluating model accuracy, each with distinct advantages. RMSE gives more importance to larger errors by squaring them, making it useful when larger errors need to be minimized. MAE, on the other hand, takes the average of all errors equally, providing a clearer measure of overall accuracy (Chugh, 2024; Chai et al., 2014). Both were used in this study to ensure the optimization improved general accuracy (MAE) while also reducing large deviations (RMSE). To determine the best α_{max} and weight set, the optimization aimed to minimize the sum of RMSE and MAE.

To evaluate the optimized model, the remaining studies from the literature review were used as the validation dataset, as listed in Table 2.5. For the validation, the optimized parameters for α_{max} and the weights were applied. The performance of the optimized model was measured using the same metrics as in the optimization phase, including RMSE and MAE. These results were then compared to the performance of the original method to determine the improvements achieved.

Tab. 2.5: Randomly picked studies from the literature review used for validation.

Validation studies					
Country	Region	Type	Soil texture	Obs.	Reference
China	Xianyang	RZWQM2	Silty loam	5	(Xu, Cai, et al., 2020)
China	Bayannaoer	APSIM	Sandy loam	3	(Ren et al., 2024)
China	Yuzhou	RZWQM2	Sandy loam	1	(Ding et al., 2020)
China	Changping	DNDC	Silty loam	3	(Y. Zhang et al., 2015)
Spain	Badajoz	APEX	Loam	7	(Chukalla et al., 2018)
China	Qiyang	Field	Sandy loam	3	(Huang et al., 2017)
China	Ya'an	Field	Sandy clay loam	8	(Yao et al., 2021)
China	Xushui	Field	Sandy loam	4	(Du et al., 2019)
Iran	Tehran	Field	Sandy loam	6	(Gholamhoseini et al., 2013)
Denmark	-	Field	Sand	6	(Simmelsgaard, 2007)

3 Results

3.1 Tier 1 python program

The Python script was validated against several published Tier 1 studies to evaluate its performance in estimating nitrogen losses using global datasets. The results, summarized in Table 3.1, provide a comparison of the α and β values derived from the Python script and the values reported in the respective studies. These comparisons reveal valuable insights into the script's accuracy and the factors contributing to any deviations.

Tab. 3.1: Results of Tier 1 case studies comparing published values with outputs generated by the automated Python program, demonstrating its performance across different locations.

Case study	Location	Study results		Python script results	
		α	β	α	β
(Muratoglu, 2020)	Turkey	0,124	0,345	0,112	0,362
(Brueck et al., 2016)	Germany	-	0,471	0,094	0,331
(Gil et al., 2017)	Colombia	0,14	-	0,128	0,386
(Rodríguez et al., 2024)	Argentina	0,128	0,42	0,136	0,446

In the case of Turkey (Muratoglu, 2020), the Python script produced an α value slightly lower than the study's result (0.112 vs. 0.124). This difference may stem from the assumptions used in the study, which adopted very conservative estimates for nitrogen fixation, application rates, and plant uptake. A key factor contributing to this deviation is the nitrogen application rate. The study capped nitrogen application at a maximum of 60 kgN/ha, while the mean N-application rate for maize in Turkey from the global dataset is 170 kgN/ha. This higher application rate increased the α by 0.08, explaining most of the observed difference. By contrast, the global dataset used in the Python script may incorporate less restrictive assumptions about nitrogen inputs, resulting in a smaller α. The β value from the script (0.362) closely matched the study's result (0.345). This close alignment reflects that β, being more dependent on environmental factors like precipitation and soil texture, exhibits less variability due to assumptions about application rates and plant uptake.

The results for Germany (Brueck et al., 2016) showed a more significant deviation in the β value, with the Python script estimating a lower value (0.331) compared to the study's reported mean (0.471). Upon further investigation, this difference can largely be attributed to an incorrect calculation of soil texture and drainage class in the study. In the original method, soil texture influences both leaching (15%) and runoff (10%), meaning that for a loam soil, leaching is assigned a value of 0.67 and runoff 0.33. However, in the study, the leaching value (0.67) was mistakenly applied to both leaching and runoff, inflating the overall leaching fraction and leading to a β value approximately 0.08 higher than expected. Second, the study assumed an N-deposition value of 1, whereas the global dataset used 0, which further increased β by 0.04. The study did not provide a specific source for this assumption but referenced general findings that nitrogen deposition is currently higher than in pre-industrial times. These factors combined suggest that the overestimated β in the study primarily stems from miscalculations in soil texture effects and an assumed higher nitrogen deposition.

For Colombia (Gil et al., 2017), the Python script estimated an α value of 0.128, slightly lower than the study's result of 0.14. Although α showed relatively good alignment, the study did not provide a β value, limiting further comparison. The close match between the two α values suggests that the estimate based on global dataset factors closely matches the estimate derived from locally determined values. However, this does not confirm the accuracy of the leaching estimate, it only confirms that the script's assumptions produce similar results to the study's calculations.

The comparison for Argentina (Rodríguez et al., 2024) demonstrated similar results as the other studies. The α values were quite similar (0.136 vs. 0.128), indicating that the global dataset used in the script aligns well with the local conditions for non-leaching nitrogen losses in this region. However, the β value estimated by the Python script was slightly higher than the study's result (0.446 vs. 0.42). This small overestimation may arise from the generalized assumptions in the script regarding precipitation, which could lead to a slightly elevated nitrogen leaching potential compared to the locally derived study values.

3.2 Tier 2 and 3 analysis

In this section, the results of the literature review are analysed to identify the key distinctions between Tier 2 and field studies compared to the Tier 1 method. By examining these differences, patterns can be uncovered that can help to improve the Tier 1 method.

The results of the literature review are illustrated in Figure 3.1, which represents the relationship between the N-leaching fraction and the N-application rate. This figure combines data points from Tier 1, Tier 2, and field studies, with separate regression lines fitted for each dataset to represent the mean of each study type.

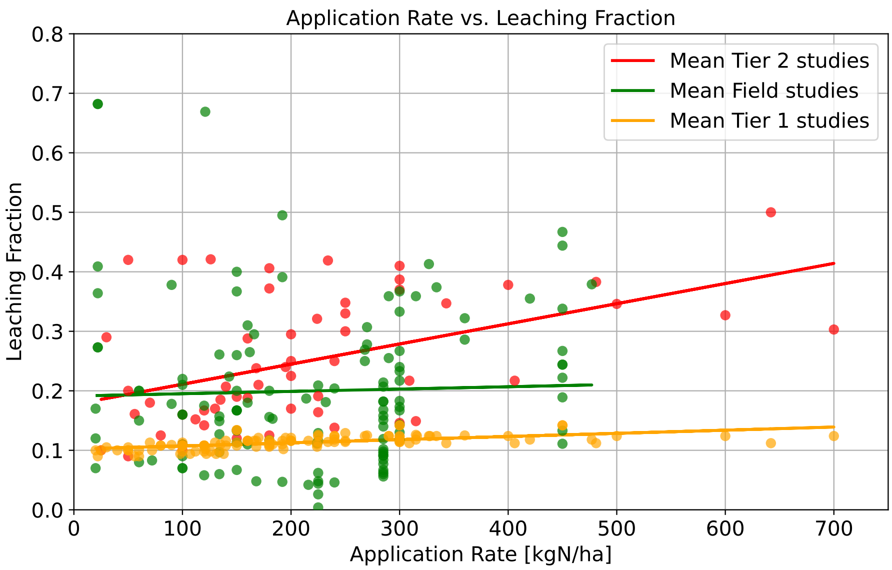


Fig. 3.1: Relationship between application rate and leaching fraction, showing the trends for Tier 1 studies, Tier 2 studies, and field studies, with all observations as colored points and the mean represented by colored lines.

The red line represents the mean trend of Tier 2 studies, which are advanced models like APEX, SWAP, RZWQM2, and DNDC. It starts at 0.19 for low application rates and rises steadily to 0.41 at the highest application rates. The upwards slope of this line indicates a positive relationship between N-application rate and N-leaching fraction, suggesting that as nitrogen application rates increase, Tier 2 studies predict a significant rise in nitrogen leaching.

The green line represents the mean trend observed in field studies, derived from real-world experiments under natural field conditions. However, the slope of the line does not show any correlation between the application rate and the leaching fraction. This could be attributed to the limited number of data points in the literature review, making it vulnerable to the influence of outliers. To address this, Figure 3.2 presents the same data categorized into bins based on the N-application rates: in steps of 50 kgN/ha up to 300 kgN/ha, followed by steps of 100 kgN/ha thereafter.

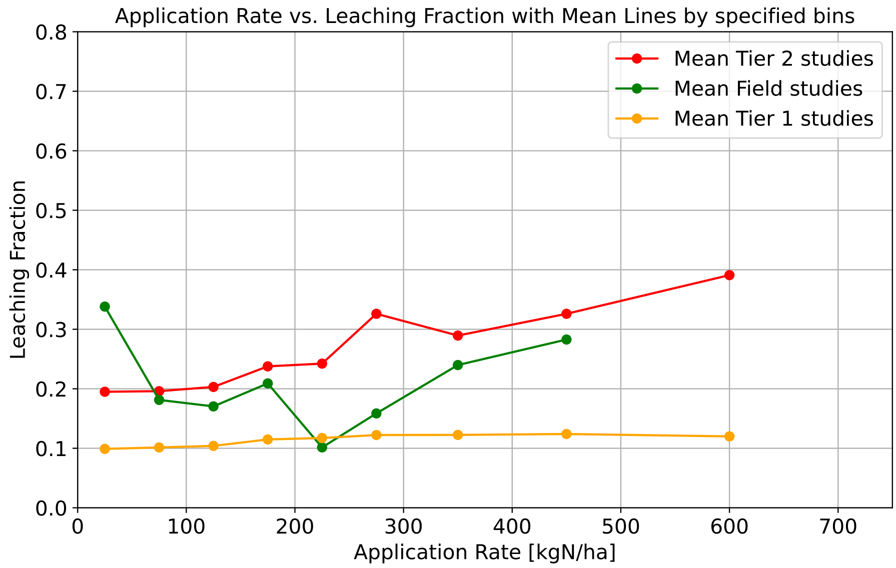


Fig. 3.2: Leaching fraction in bins to show study variability.

In the binned analysis in Figure 3.2 the green line initially starts high at 0.35 for application rates between 0 and 50 kgN/ha. This is due to the findings of Sogbedji et al. (2000), which indicate that in this field study at low N-application rates, high residual nitrogen in the soil and the presence of sandy soil contribute to an increased leaching fraction. From 50 to 450 kgN/ha there is a gradual increase in the N-leaching fraction from 0.18 to 0.28, except for a notable dip in the range of 200 to 250 kgN/ha. This can be attributed to findings from (Fan et al., 2017), where nitrogen losses were reported for different fertilizer types at a fixed application rate of 225 kgN/ha. Compared to other field studies the reported losses were remarkably low, ranging from 0.001 to 0.05 for maize. This was likely due to the clayey soil texture, which inherently prevents high leaching losses. Overall, the field studies reveal an increasing trend in nitrogen leaching fraction with higher application rates, though the slope is somewhat less steep than the Tier 2 line.

The orange line in Figure 3.1 & Figure 3.2 represents the Tier 1 method conducted in the same locations as the Tier 2 and field studies, but unlike them, the Tier 1 line has a much flatter slope, indicating only a slight increase in leaching fraction from 0.1 to 0.13 at higher application rates. This suggests that Tier 1 studies may consistently underestimate nitrogen leaching compared to both field and Tier 2 studies, especially at higher nitrogen application rates.

The scatterplot in Figure 3.3 shows all Tier 2 and field study data points on the x-axis plotted against their corresponding Tier 1 values on the y-axis. This figure highlights the greater variability observed in Tier 2 and field studies compared the Tier 1 method. Unlike Figure 3.1, which focuses on the mean values, this scatterplot shows the lack of alignment in a clearer way.

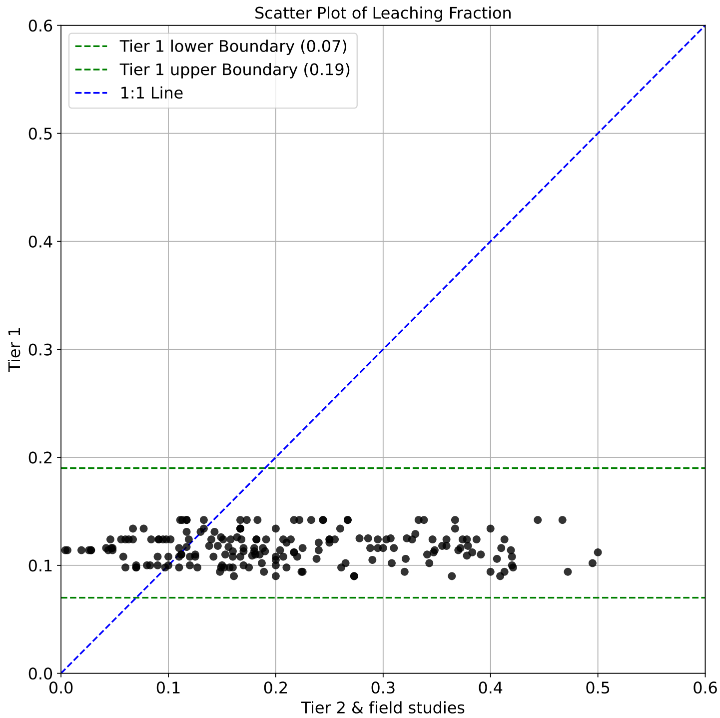


Fig. 3.3: Comparison of Tier 1 and Tier 2 leaching fractions from the literature review, with the 1:1 line indicating perfect agreement between the two tiers.

The leaching fractions for the Tier 1 method studies are tightly clustered and concentrated between 0.1 and 0.15, constrained by the boundaries (0.07 - 0.19) of the equation, this narrow range indicates a relatively consistent but low leaching rate across these data points and shows low variability in the method. This clustering suggests that the Tier 1 methodology, even across different studies, produces similar leaching fraction estimates, which may indicate potential methodological limitations that do not fully capture variations in nitrogen leaching across different conditions.

In contrast, the Tier 2 and field study data points show a much wider spread, ranging from 0 up to 0.5. This suggests that Tier 2 studies capture more variability and, on average, report higher leaching fractions. Tier 2 methods, possibly due to greater sensitivity or model complexity, are observed to be more responsive to environmental factors that impact nitrogen leaching.

The significant differences between Tier 1 and the other study types suggest that relying solely on Tier 1 could lead to an underestimation of nitrogen leaching, potentially resulting in recommendations for nitrogen applications that exceed what the environment can safely tolerate.

3.3 Identifying key factors in Tier 1

This section presents the results of the evaluation of the Tier 1 method. To assess the method, a sensitivity analysis of the Tier 1 method is conducted. This isolate the influence of individual factors on the leaching fraction, identifying the most significant contributors to variability within the Tier 1 method. This analysis not only highlights the method's strengths and limitations but also pinpoints areas where adjustments could improve its alignment with the Tier 2 method.

The results of the sensitivity analysis from the case study by Choruma et al. (2021) are shown in Figure 3.4. The blue line in the figure represents the original leaching fraction value of 0.129, calculated using the Tier 1 method, and serving as the baseline for the analysis. The red lines indicate the boundaries of the Tier 1 method: the minimum leaching fraction of 0.07 and the maximum of 0.19. For comparison, the Tier 2 study in the case study, based on a N-application rate of 250 kgN/ha, reported a leaching fraction of 0.33.

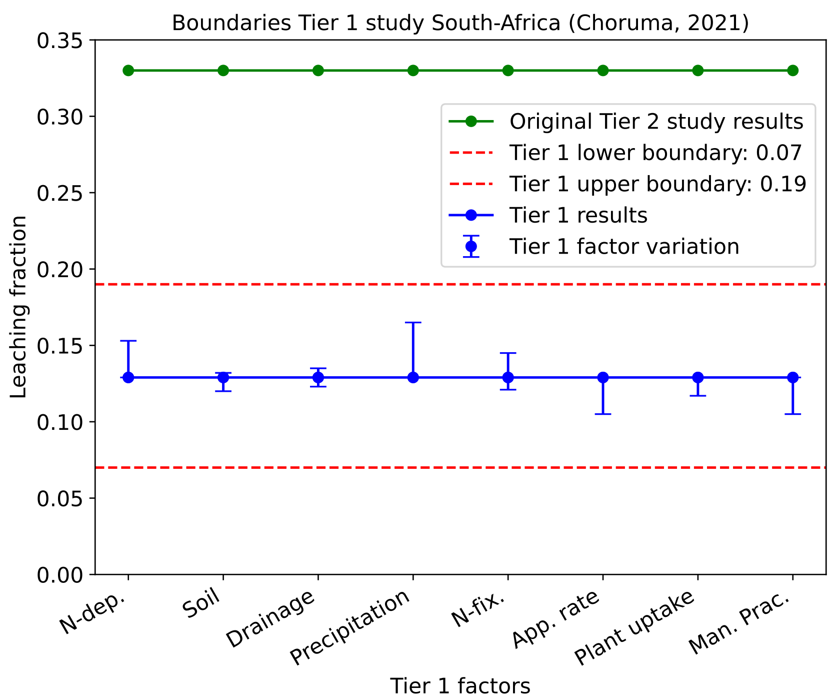


Fig. 3.4: Tier 1 method range bar per factor, shown alongside Tier 1 boundary and original Tier 2 study results.

Each factor is represented with a range bar in the figure, showing the variability in leaching fraction when that specific factor is varied between 0 and 1. A wider range bar indicates a greater influence of the factor on the leaching fraction.

The results of Figure 3.4 are quantified in Table 3.2, which highlights the range of each factor in the Tier 1 method. Among these factors, precipitation is identified as the most influential, in this case study the annual precipitation is below 600 mm, so a score of 0 is given, but would this have been a location where it rains more than 1800 mm annually the leaching fraction would be increased by 0.036. The significant impact is attributed to the 15% weight assigned to precipitation in the Tier 1 method, although it is not the highest weighted factor.

The highest weights are assigned to soil texture (25%) and drainage classes (20%). However, their influence is considerably lower than that of precipitation, with a range of only 0.012 each. This reduced impact arises from the factors being divided between promoting leaching and runoff. For instance, sandy soils, which allow rapid water infiltration, receive a high leaching score (1) but a low runoff score (0). This balancing effect decreases their overall contribution to the leaching fraction, despite their high weights.

Tab. 3.2: Ranges of influence of each Tier 1 factor on the N-leaching fraction.

Tier 1 factor	Range
N-deposition	0.024
Soil texture	0.012
Drainage class	0.012
Precipitation	0.036
N-fixation	0.024
Application rate	0.024
Plant uptake	0.012
Management practices	0.024

Other factors, including nitrogen deposition, nitrogen fixation, application rate, and management practices, also contribute to the leaching fraction but are less impactful compared to precipitation, with ranges at 0.024. This indicates that while these factors contribute to nitrogen dynamics, their effects are more consistent and do not result in the same level of variability seen with precipitation.

Of all the factors, the application rate is the most suitable factor for improving the Tier 1 method. It is a key contributor to nitrogen leaching and has significantly higher data availability to other factors. Unlike precipitation, soil texture, and drainage class, which are static and region-specific values, the application rate is dynamic and can vary significantly even within the same region. Furthermore, factors such as nitrogen deposition, nitrogen fixation, and management practices are either influenced by external environmental conditions or too complex to isolate for effective optimization. The application rate's flexibility, impact, and practicality make it the ideal choice for improving the Tier 1 method.

To address the underestimating of nitrogen leaching in the Tier 1 method, several adjustments were tested, focusing on modifying specific factors within the equation. The first adjustment was the weight assigned to the nitrogen application rate, which was originally set at 10%, resulting in a leaching fraction of 0.129 for high application rates in the study of Choruma et al. (2021). The aim was to determine whether increasing this weight could improve the model's prediction. As shown in Table 3.3, even when the weight factor was increased to the maximum level of 55%, where all the other factors are 5%, then leaching predicted by Tier 1 only increased from 0.129 to 0.194, which still fell far short compared to the Tier 2 predictions of 0.33. This demonstrates that modifying the weight of the application rate alone is insufficient to resolve the underestimation issue.

The leaching fraction at 100 kgN/ha does not follow a consistent increasing trend, showing small fluctuations as the weight factor changes. This variation is caused by the redistribution of the weight of the other factors. As the application rate weight increases, the contributions from other factors decrease at different rates, leading to minor deviations in the final leaching fraction. In this case study, some factors have a value of 1, meaning they have a stronger influence when the weight of that specific factor is downgraded. When factors with lower values are downgraded, they contribute less to the overall calculation, which can cause the leaching fraction to remain stable rather than increasing as expected.

Tab. 3.3: effect of varying weights of application rate on leaching fractions under normal and high application rates.

Weight of application rate	Leaching fraction (100 kgN/ha)	Leaching fraction (250 kgN/ha)
10% (normal)	0.113	0.129
20%	0.117	0.141
30%	0.113	0.161
40%	0.109	0.173
50%	0.102	0.182
55%	0.106	0.194

The fundamental issue appears to be the maximum leaching fraction (α_{max}) applied within the Tier 1 method, which is 0.25. This has a significant impact on the overall equation because it creates a maximum boundary of 0.19, essentially limiting the potential leaching that could be predicted at higher application rates. To address this, the next test involved increasing α_{max}, allowing the equation to better reflect conditions of elevated nitrogen inputs. The results of this test for very high and low

N-application rates are shown in Table 3.4. The adjustment of α_{max} showed the most promise, producing results close to those of the Tier 2 method when an α_{max} of more than 0.625 is used.

However, increasing the α_{max} has the side effect of elevating the entire equation, leading to an overestimation at lower application rates. Additionally, further reducing α_{min} is unlikely to resolve this issue, as it is already set at only 1%, meaning the lower boundary is already near the lowest possible leaching levels. The optimal solution would likely involve selecting an α_{max} value between 0.25 and 1, combined with adjustments to the weight of the application rate, to achieve a balance that accurately reflects leaching across the full range of conditions.

Tab. 3.4: Effect of varying α_{max} values on leaching fractions under high and low N-application rates.

α_{max}	Leaching fraction (250 kgN/ha)	Leaching fraction (50 kgN/ha)
0.25 (normal)	0.129	0.105
0.375	0.191	0.154
0.50	0.253	0.204
0.625	0.315	0.253
0.75	0.377	0.303
0.875	0.439	0.352
1	0.501	0.402

3.4 Optimization

In this section the results of the optimization of α_{max} and the weight of the N-application rate are reported. The objective of the optimization was to reach the lowest sum of RMSE and MAE as possible. For each weight set a new optimization was conducted that came with its own α_{max}. This approach was necessary because it allowed α_{max} to adjust with the changing weight, this led to a lower RMSE and MAE, improving the overall model fit.

Table 3.5 presents the optimization results for all the predefined weight sets, summarizing the key metrics. The table includes the optimal α_{max} for each weight set, the evaluation scores (Root Mean Square Error, RMSE, and Mean Absolute Error, MAE).

Tab. 3.5: Optimization results for each weight set, including α_{max} and evaluation scores.

Weight set		α_{max}	Scores		
			RMSE	MAE	Sum
1.	10%	0.250	0.166	0.121	0.287
2.	15%	0.495	0.134	0.114	0.248
3.	**20%**	**0.475**	**0.133**	**0.114**	**0.247**
4.	25%	0.475	0.135	0.115	0.250
5.	30%	0.452	0.135	0.115	0.250
6.	35%	0.439	0.136	0.115	0.251
7.	40%	0.430	0.138	0.116	0.254
8.	45%	0.433	0.140	0.117	0.257
9.	50%	0.443	0.141	0.117	0.258
10.	55%	0.420	0.141	0.117	0.258

The scores, RMSE and MAE, represent the model's predictive accuracy, with lower values indicating better performance. Weight set 3, which assigns 20% weight to the N-application rate in combination with an optimized α_{max} of 0.475, was selected as the most optimal configuration because it achieved the lowest combined RMSE and MAE. Specifically, it produced the lowest RMSE (0.133) and MAE (0.114) among all tested weight sets. Compared to the original method, this optimization led to a 20% reduction in RMSE (from 0.166 to 0.133), and the MAE also decreased by 6% (from 0.121 to 0.114).

In Table 3.6 two sets of boundary values are shown. The low, high, and range columns represent the possible value range of the new Tier 1 method, defining the theoretical limits within which the new method can operate. The minimum, maximum, and range columns refer to the actual observed value range for the specific cases considered in the optimization.

Tab. 3.6: Theoretical method boundaries and optimization case study boundary ranges for each optimized weight set.

Weight set		Theoretical method boundaries			Optimization results		
		Low	High	Range	Min.	Max.	Range
1.	10%	0.070	0.190	0.120	0.090	0.142	0.052
2.	15%	0.131	0.374	0.243	0.160	0.281	0.121
3.	**20%**	**0.126**	**0.359**	**0.233**	**0.154**	**0.285**	**0.131**
4.	25%	0.126	0.359	0.233	0.138	0.300	0.162
5.	30%	0.121	0.342	0.221	0.132	0.308	0.178
6.	35%	0.096	0.353	0.257	0.117	0.317	0.200
7.	40%	0.094	0.346	0.252	0.104	0.321	0.217
8.	45%	0.095	0.348	0.253	0.095	0.327	0.232
9.	50%	0.075	0.378	0.303	0.089	0.334	0.245
10.	55%	0.072	0.359	0.287	0.085	0.331	0.246

The optimization results demonstrate a significant expansion in the method's boundaries, with the theoretical range nearly doubling from 0.120 to 0.233. This increase is driven by a rise in the upper boundary from 0.190 to 0.359, while the lower boundary also shifts upward from 0.070 to 0.126. When the Tier 1 method is applied to Tier 2 case studies, the original values range from 0.090 to 0.142, but under the optimized method, this range increases to 0.154 and 0.285. In comparison, the original Tier 2 values span a much wider range, from 0.004 to 0.682, making direct comparison challenging.

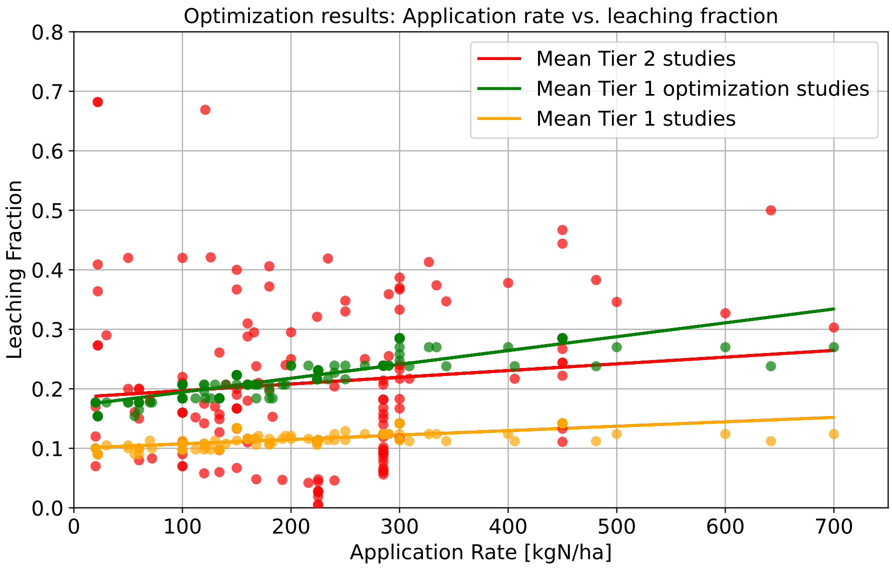
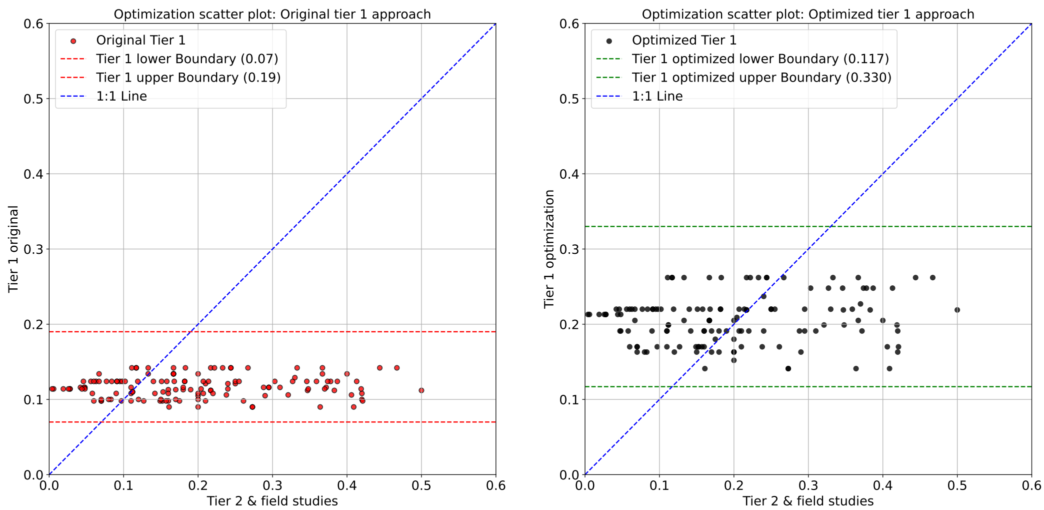


Fig. 3.5: Optimization results showing the relationship between application rate (kgN/ha) and leaching fraction, comparing mean values from Tier 2/field studies, optimization Tier 1, and original Tier 1 values.

Figure 3.5 compares the mean leaching fraction of the original Tier 1, Tier 2/field studies and the optimized Tier 1. The optimized model with an α_{max} of 0.475 and a weight of 20 % achieves a close alignment with the mean of the Tier 2 and field studies. All data points of the optimization fall within the range of 0.154 and 0.285. In contrast, the original method has narrower boundaries of 0.090 to 0.142.

The scatter plots in Figure 3.6 presents the relationship between the Tier 1 values and the observed Tier 2 and field study values, where Figure 3.6a shows the original method's results and Figure 3.6b shows the optimized method's results. This figure provides a more nuanced view of the optimized Tier 1 method's performance. The optimized Tier 1 values generally cluster closer to the 1:1 line than the original method, particularly in the range of 0.15 to 0.30. However, notable deviations remain, especially for lower leaching fractions (0 to 0.15), where the optimized method overestimates values. This indicates that the optimization process could not fully capture the observed patterns.



(a) Scatterplot original Tier 1 method vs. Tier 2/field studies

(b) Scatterplot optimized Tier 1 method vs. Tier 2/field studies

Fig. 3.6: Scatterplot comparison between original and optimized Tier 1 method

While the optimization significantly reduces RMSE and MAE, it is constrained by the variability of the input data and the simplicity of the Tier 1 approach. Figure 3.5 reveals that while general trends are well captured, predicting individual data points across diverse case studies remains a challenge as shown in the scatter plots in Figure 3.6.

3.4.1 Validation

The validation results, presented in Figure 3.7, demonstrate similar outcome to the optimization phase. The mean line of the optimized Tier 1 values initially starts below Tier 2 and field study values but surpasses them at higher application rates. However, it is important to note that this dataset lacks data points above 500 kgN/ha, resulting in a shorter trend line compared to the optimization results.

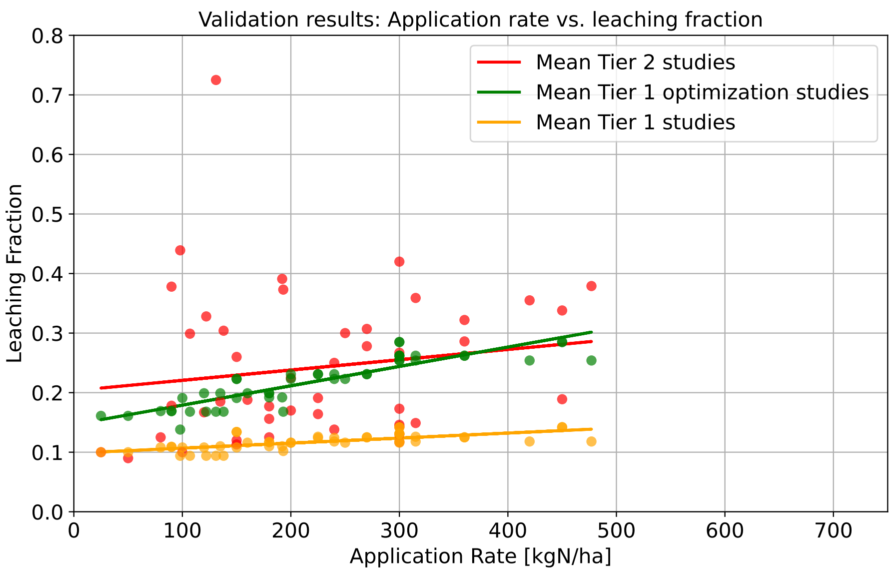
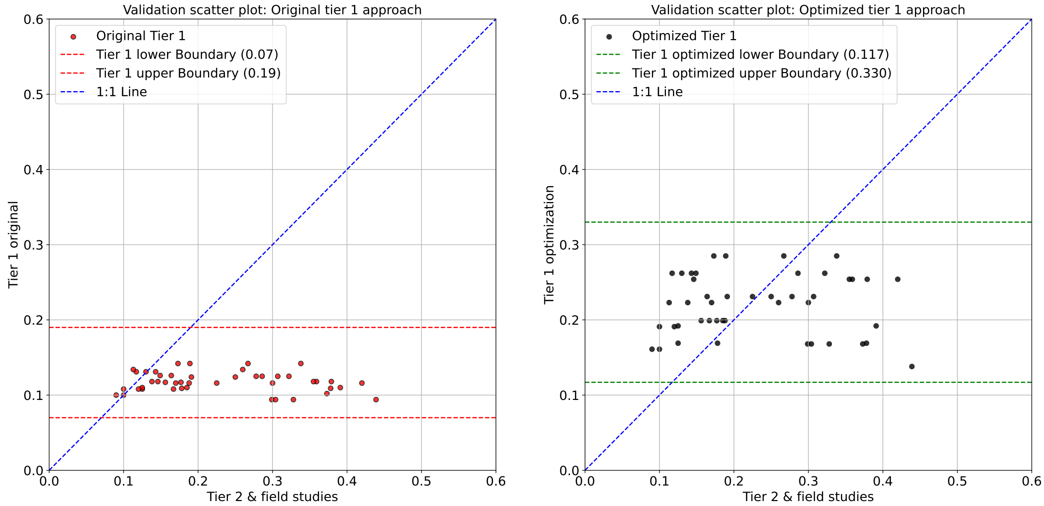


Fig. 3.7: Validation results showing the relationship between application rate (kgN/ha) and leaching fraction, comparing mean values from Tier 2/field studies, optimization Tier 1, and original Tier 1 values.

Figure 3.8 presents the relationship between the optimized Tier 1 values and the observed Tier 2 values in a scatterplot. Figure 3.8a presents the original method's results, which yielded an RMSE of 0.178 and an MAE of 0.127, while Figure 3.8b displays the optimized method's results, which improved to an RMSE of 0.135 and an MAE of 0.098. As summarized in Table 3.7, the optimization led to a 20% reduction in RMSE and a 6% improvement in MAE during the optimization phase, while validation saw even greater improvements of 24% and 23%, respectively.

Tab. 3.7: Comparison of RMSE and MAE for the original and new methods in optimization and validation.

	Optimization		Validation	
	RMSE	MAE	RMSE	MAE
Original method	0.166	0.121	0.178	0.127
New method	0.133	0.114	0.135	0.098
Improvement (%)	20	6	24	23



(a) Original Tier 1 Approach

(b) Optimized Tier 1 Approach

Fig. 3.8: Comparison of Tier 1 Approaches

Despite these improvements, visual observations indicate a greater spread in the validation phase, with a noticeable overestimation of leaching fractions in the 0.1–0.2 range. This range represents a significant portion of the dataset, but there is a wide array and random variability in application rates. this complicates further adjustments to the optimized method, as any modification risks negatively affecting model performance in regions where it already aligns well. Similarly, reducing α_{max} could lower predictions across all data points, potentially decreasing the RMSE and MAE, but failing to specifically address the overestimation in this dataset. This highlights the inherent trade-offs in the optimization process, where global parameters affect the entire dataset, limiting the model's ability to target specific regions without introducing new errors elsewhere.

Discussion

4

4.1 Tier 1 Python script

While the python script produced results that aligned reasonably well with published values in some cases, significant challenges and limitations emerged during its application, which impacted the reliability and efficiency of the process. These challenges highlight areas for improvement in the script and dataset choices.

The initial goal was to develop a fully automated Tier 1 method. However, this proved to be unreachable due to several obstacles, still demanding manual inputs into certain parts. A key limitation was the inability to automate the soil texture and drainage class data. Currently, these values must be manually taken from the HWSD 2.0 viewer. This manual process arises because the underlying data used by the viewer is difficult to access in a format that allows for an integration with python, and the data structure makes it challenging to retrieve the correct information solely based on input coordinates.

Another significant challenge was the reliance on global datasets for N-application rates, N-fixation and plant uptake. The dataset used provides values at a national level rather than at a high spatial resolutions. This lack of spatial resolution proved problematic, particularly in larger countries, where N-application rates can vary widely across regions. While this limitation did not significantly affect the results of this study, since the application rates from Tier 2 and field studies were used, future research focused solely on deriving Tier 1 values for specific regions would greatly benefit from datasets with finer spatial resolution to improve accuracy.

4.2 Literature review

One of the primary reasons the optimization process did not achieve ideal results is the limited size and diversity of the literature review dataset. In the end, the dataset lacked representation from a wider range of regions globally, which is essential for capturing the variability in the environmental factors that influence nitrogen leaching. The dataset was dominated by loam soils, which also meant that drainage class was mostly moderately well-drained, limiting variability in this factor. Precipitation levels were generally low, with few studies from higher-rainfall regions, making it difficult to assess the impact of wetter conditions. Additionally, some data, such as management practices, nitrogen fixation, and plant uptake, were reported at the national level, reducing differentiation, especially in large countries with diverse agricultural conditions, such as China. Plant uptake was also not crop-specific, further limiting variability. These limitations will be explored in more detail in section 4.4.

The challenges began during the literature review, primarily due to insufficient attention to the variety of terminology used in nitrogen leaching studies. While terms like: "leaching rate", "leaching loss", "leaching fraction" and "leaching ratio" were included in the search, the variability in terminology may have resulted in the exclusion of relevant studies. Many papers may not explicitly use these terms or may focus on only one component without combining them. This lack of standardization in the terminology complicated the process of identifying all relevant literature. Expanding the scope to include additional synonyms such as "leachate," "leakage," "leaching flux," "percolation," and "seepage," along with related concepts, could have improved the literature review.

Additionally, focusing solely on maize further narrowed the pool of studies. While maize is a common and widely studied crop, this restriction excluded research on other crops that could have provided valuable insights into nitrogen leaching under different conditions. Expanding the scope to include other major crops, such as wheat, rice, and soybeans, could help determine whether the observed trends in nitrogen leaching hold across different crop types. Similarly, beyond nitrogen leaching, the applicability of the optimized method to other pollutants such as phosphorus or other pesticides remains uncertain. Testing the optimized method against these pollutants would help determine whether the optimized method remains robust or if modifications are needed for other pollutants to account for different contaminant behaviors.

Another challenge is that including Tier 2 model names, such as DSSAT, in the search terms for the literature review does not effectively yield relevant studies on nitrogen leaching. While this approach generates a large number of search results, most of these studies use the models for broader agricultural or environmental analyses, where nitrogen leaching is only a secondary outcome rather than the primary focus. As a result, many of the retrieved papers lack the necessary details, such as nitrogen application rates or direct leaching estimates, making them unsuitable for inclusion in the dataset. This limits the usefulness of model-based keyword searches.

4.3 Linear model limitations

A fundamental limitation of the Tier 1 method is that it assumes a linear relationship between nitrogen application, environmental factors, and leaching, whereas nitrogen leaching in reality follows nonlinear patterns and involves complex interactions. This makes it challenging to calibrate the Tier 1 method using field data and Tier 2 studies, as these naturally capture nonlinear effects. While the optimized method improves performance by adjusting key parameters, the linear nature of Tier 1 still restricts its ability to fully reflect nitrogen leaching under different conditions.

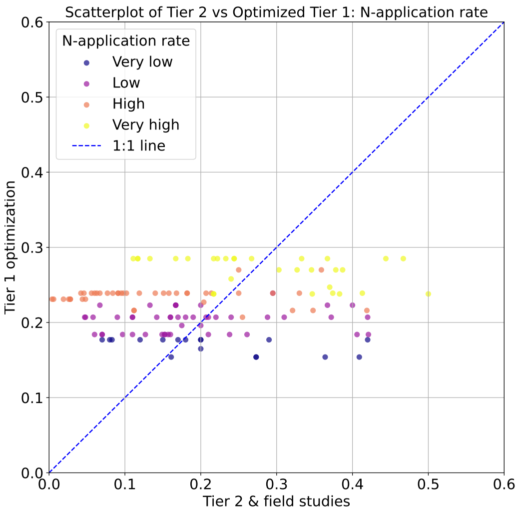
Calibrating a linear model with nonlinear field and Tier 2 data presents several challenges. One of the main issues is that nitrogen leaching does not respond proportionally to changes in nitrogen application, precipitation, or other environmental factors. In reality, leaching does not always start low. In some cases, it is already high at low nitrogen levels, depending on soil and plant uptake. As nitrogen input increases, leaching can rise even more sharply when the retention capacity is exceeded. A linear model such as the Tier 1 method cannot capture this shift, often underestimating leaching at high nitrogen levels and overestimating it at low nitrogen levels. As a result, fitting a straight-line model to nonlinear data forces a compromise across the dataset, introducing bias that affects accuracy.

Another difficulty arises from how the Tier 1 method handles precipitation. Instead of accounting for short-term heavy rainfall events, which cause most nitrogen losses, Tier 1 relies on annual precipitation. However, nitrogen leaching is highly event-driven, occurring primarily when rainfall exceeds soil infiltration capacity. Two regions with the same total precipitation may have very different leaching risks, depending on whether rainfall is evenly distributed or occurs in extreme storms. Since the linear model applies a fixed leaching rate, it cannot capture sudden spikes in nitrogen loss after storms, making calibration with field and Tier 2 data difficult. These limitations highlight why Tier 1 calibration remains constrained, even after optimization.

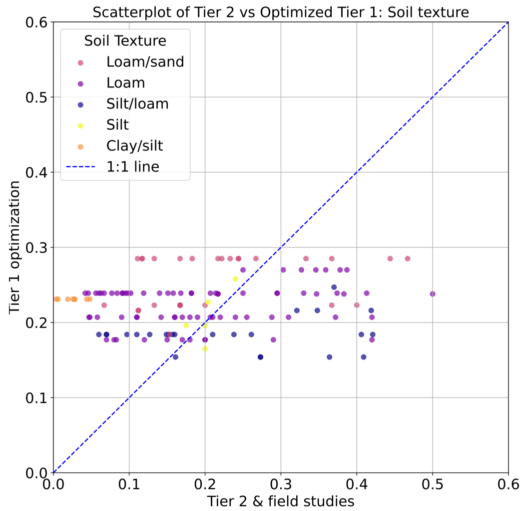
4.4 Variability per factor

A reason why the optimization process could not fully capture the observed patterns is the variability in leaching fractions for different factors in the Tier 2 and 3 studies, which is visualized in Figure 4.1 to Figure 4.4, where scatterplots show the spread of values for each distinct range (very low, low, high, and very high), with Tier 1 plotted on the y-axis and Tier 2/3 on the x-axis.

In Figure 4.1a, the variability of the application rate factor between Tier 1 and Tier 2/3 is illustrated. In Tier 1, clear color-segmented groupings appear along the y-axis due to the categorical nature of the scoring system of Tier 1. A very high application rate (yellow) contributes heavily to the calculation, clustering these points at the top. Conversely, a very low application rate results in lower leaching fractions, leading to a clear segregation between the four score categories (very low, low, high, and very high). However, in Tier 2/3, no apparent relationship exists between application rate and leaching fraction, as individual data points are more scattered across the x-axis. This suggests that on a basis of individual data points leaching fraction in Tier 2/3 is not solely influenced by application rate, this differs from the case in the mean trend analysis of these data points where the application rate seemed more important. This could mean that other factors also play a significant role in determining leaching fraction in Tier 2/3 models, and suggest that in further refinements, other factors should be given greater attention to improve accuracy.



(a) Application rate

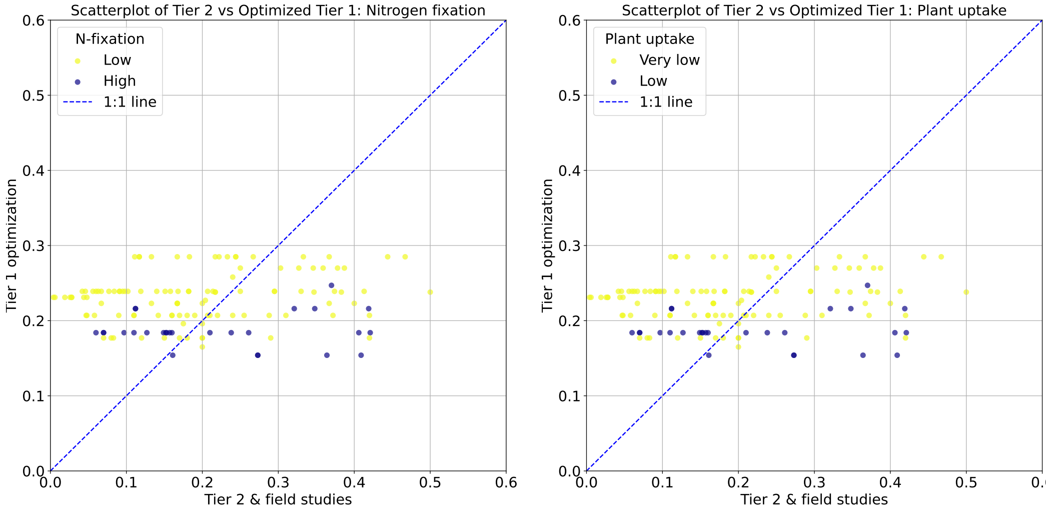


(b) Soil texture

Fig. 4.1: Variability in the leaching fraction as influenced by application rate and soil texture.

In Figure 4.1b, the variability in soil texture is examined. Studies involving loam/sand (pink), loam (purple), and silt/loam (blue) textures reveal a considerable spread in leaching fraction along both axis, while silt (yellow) clusters around 0.2 for both methods. A notable mismatch appears in the clay/silt (orange) texture, where Tier 2 values remain very low, whereas Tier 1 values approach 0.25. However, these observations are limited by the fact that each texture category that shows clustering is represented by only a single study.

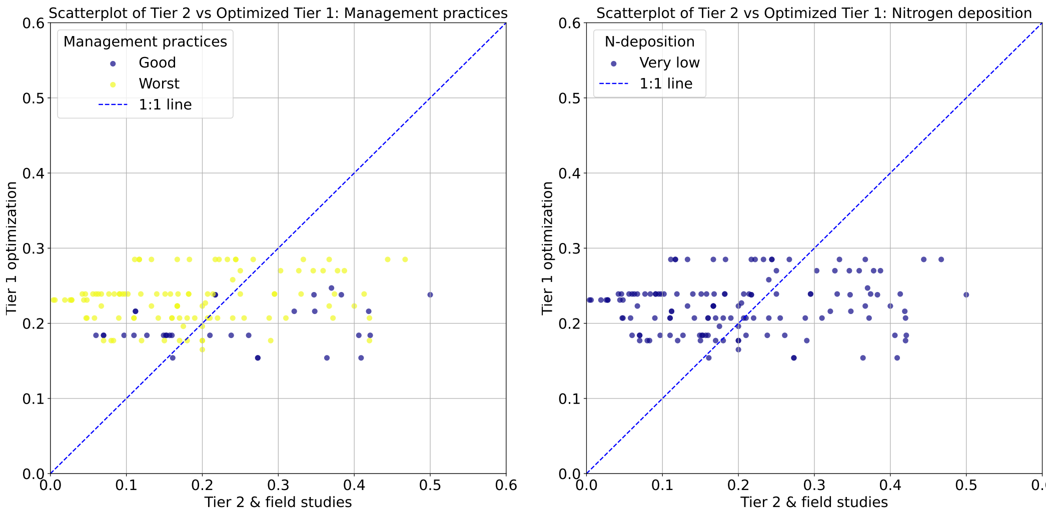
While application rate and soil texture displayed some degree of variability, other factors showed minimal variability, limiting their usefulness for further analysis for now because of the lack of data availability in this thesis. With more Tier 2/3 data in future research, a more detailed analysis will be possible. The leaching fractions



(a) Nitrogen fixation **(b)** Plant uptake

Fig. 4.2: Variability in the leaching fraction as influenced by nitrogen fixation and plant uptake.

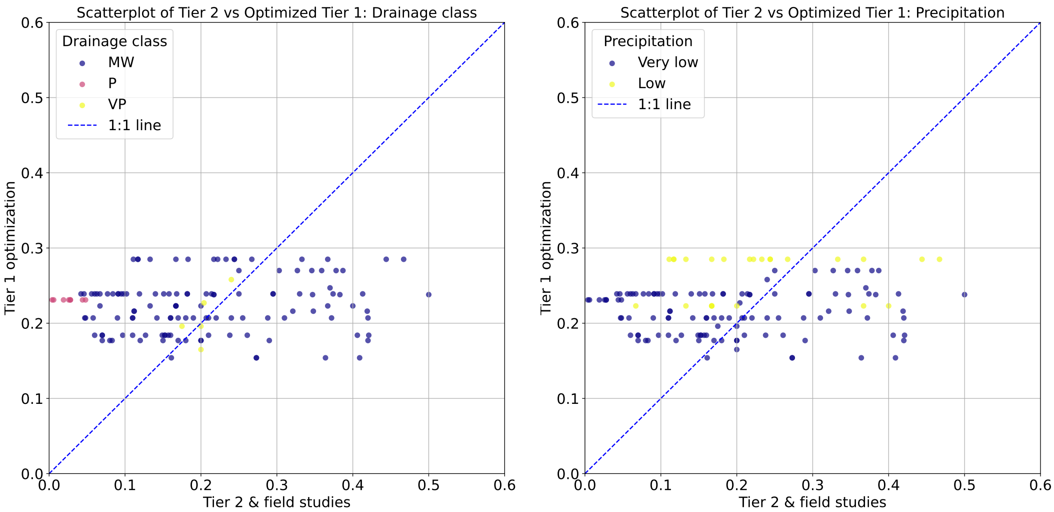
for nitrogen fixation (Figure 4.2a), plant uptake (Figure 4.2b), and management practices (Figure 4.3a) remained largely uniform. This lack of variation can be attributed to the datasets used, which reported values at a national level, reducing the differentiation between data points. Additionally, a large portion of the data used in the optimization originated from China, contributing to the uniformity in these factors.



(a) Management practices **(b)** Nitrogen deposition

Fig. 4.3: Variability in the leaching fraction as influenced by management practices and and nitrogen deposition.

For nitrogen deposition (Figure 4.3b), no clear patterns emerge along either axis, with all data points falling within a single range. This could indicate an issue with the dataset or that the defined ranges are not appropriately set. The classification for nitrogen deposition defines values below 0.5 g N $m^{-2}yr^{-1}$ as very low, 0.5–1 as low, 1–1.5 as high, and above 1.5 as very high. For drainage class (Figure 4.4a), nearly all data points fall within the "moderately well-drained" category, with only one study classified as "poorly drained" and another as "very poorly drained." This is not due to limitations in the HWSD dataset, which includes various drainage classes, but rather a lack of representation in the literature review data. Similarly, precipitation (Figure 4.4b), despite being derived from coordinates with a reasonable spatial resolution of 278 km^2, is predominantly below 600 mm annually across nearly all studies. As with drainage class, this appears to be a matter of limited study locations rather than a data issue. The lack of diversity in the types of studies used prevented strong conclusions from being drawn about the relationship between these three factors and the leaching fraction.



(a) Drainage class

(b) Precipitation

Fig. 4.4: Variability in the leaching fraction as influenced by drainage class and precipitation.

A missed opportunity in this study was conducting the factor analysis only after the optimization process, rather than during the dataset gathering stage of the literature review in the second research question. The lack of variability in most factors was only recognized too late in the process. Early identification of these limitations could have informed a more targeted search strategy to include a broader range of studies, particularly from the underrepresented regions and environmental conditions. Future research should first conduct a broad literature review to compile an initial dataset, followed by an exploratory factor analysis to assess variability in key factors. If the analysis reveals insufficient representation of certain regions, crops, or soil types, a more targeted literature search should be performed to address these gaps and ensure a more balanced dataset.

5 Conclusion

This thesis aimed to refine the Tier 1 nitrogen leaching-runoff estimation method to narrow the accuracy gap between the Tier 1 and Tier 2 method, while maintaining the simplicity and lower data requirements of Tier 1. The refined and automated Tier 1 method developed in this study provides a more user-friendly and accurate tool for assessing nitrogen leaching than the original Tier 1 method of Franke et al. (2013). However, the Tier 1 method's value in supporting sustainable nitrogen management remains limited by its inability to accurately capture results from advanced models or field experiments.

While the refined method is a more practical tool for assessing nitrogen leaching, its value in supporting sustainable nitrogen management depends on improving its sensitivity to nitrogen application rates. Without such improvement, the method may still lead to conclusions where environmental impacts are not adequately reflected, making economic factors the primary driver in nitrogen application decisions.

The development of a Python-based automated Tier 1 script streamlined the traditionally manual process of data collection and calculation. By using global datasets, the script eliminates the need for extensive manual labor typically required to gather site-specific data, saving significant time and enabling the analysis of multiple locations quickly. This makes it a reliable and scalable solution for broad-scale evaluations of nitrogen leaching. While the script relies on generalized assumptions, its comparison with other Tier 1 studies demonstrated that it achieves reasonable accuracy, even when compared to other Tier 1 studies based on highly localized data. This balance between practicality and accuracy ensures its effectiveness for large-scale applications, despite minor deviations caused by its generalized approach.

While the script significantly reduces manual effort, it still depends on both automated and manual data inputs. Nitrogen deposition, precipitation, nitrogen fixation, plant uptake, and nitrogen application rates are efficiently retrieved from global datasets, but soil type, drainage class, and management practices require manual input due to the lack of a suitable dataset. The full implementation and dataset details can be accessed at Zenedo (Scholten, 2025).

A detailed analysis of Tier 2 and field studies provided valuable insights into the limitations of the original Tier 1 method. Compared to Tier 2 models and field studies, the original Tier 1 method was found to consistently underestimate nitrogen leaching, particularly at higher nitrogen application rates when the mean of multiple studies was considered. The analysis revealed that Tier 2 studies captured greater variability by incorporating dynamic environmental and management factors, which Tier 1 oversimplified. This understanding informed the refinement process, highlighting the need for greater variability and flexibility in Tier 1 calculations.

Through the evaluation of individual factors, the method was refined to better account for the most influential variables, particularly precipitation and nitrogen application rate. Optimizing the nitrogen application rate proved to be the most practical approach due to its high data availability, allowing for systematic adjustments. In contrast, the complexity of precipitation as a variable made it more challenging to implement substantial methodological changes.

The optimization process improved the Tier 1 method. By increasing the maximum leaching fraction (α_{max}) from 0.25 to 0.475 and raising the weight assigned to the nitrogen application rates from 10% to 20%, the refined Tier 1 method achieved a 25% reduction in the selected predictive error metrics (RMSE & MAE). This adjustment also expanded the boundary range, enabling the method to capture greater variability in nitrogen leaching across different conditions.

While the refined approach aligned more closely with Tier 2 and field study results when comparing the mean across multiple studies, it showed significant limitations in accurately predicting individual data points. These limitations, particularly in its sensitivity to nitrogen application rates, suggest that the model may not be reliable for precise, localized predictions. It is also difficult to argue that the model is useful for broad-scale assessments, such as identifying general trends in countrywide or global nitrogen leaching, when this thesis demonstrates that higher leaching fractions are not driven by increases in nitrogen application rates.

To further refine the Tier 1 method, future research should focus on expanding the literature review to incorporate a broader and more diverse range of studies. A key limitation in this study was recognizing the lack of variability in certain factors only after the optimization process, rather than during the dataset gathering stage. Conducting an exploratory multi factor analysis early in the literature review phase would help identify gaps in regional representation, crop types, and environmental conditions, enabling a more targeted search strategy to build a more balanced dataset. By incorporating this data, the influence of the N-application rate across Tier 2 and 3 studies or other factors can be better differentiated. While increasing α_{max} improved accuracy, it introduces the potential for overestimation in scenarios with low nitrogen application rates. Additionally, the automation of the soil texture and the drainage class from the HWSD 2.0 viewer would be a valuable improvement. Combining this with well-designed approach to quantify the management practice factor and a higher spatial resolution dataset for N-fixation, plant uptake and application rate would complete the script.

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Appendix

Tier 1

Category	Factor		Nitrogen					
			Leaching-runoff potential		Very low	Low	High	Very high
			Score (s)		0	0.33	0.67	1
			Weight* (w)					
			α	β				
Environ-mental factors	Atmos-pheric input	N-deposition (g N $m^{-2}yr^{-1}$) (see Appendix II Map 1)	10	10	< 0.5	> 0.5	< 1.5	> 1.5
	Soil	Texture (relevant for leaching) (see Appendix II Map 2)	15	15	Clay	Silt	Loam	Sand
		Texture (relevant for runoff) (see Appendix II Map 2)	10	10	Sand	Loam	Silt	Clay
		Natural drainage (relevant for leaching) (see Appendix II Map 3)	10	15	Poorly to very poorly drained	Moderately to imperfectly drained	Well drained	Excessively to extremely drained
		Natural drainage (relevant for runoff) (see Appendix II Map 3)	5	10	Excessively to extremely drained	Well drained	Moderately to imperfectly drained	Poorly to very poorly drained
	Climate	Precipitation (mm) (see Appendix II Map 5)	15	15	0-600	600-1200	1200-1800	> 1800
Agricul-tural practice	N-fixation (kg/ha)		10	10	0	> 0	< 60	> 60
	Application rate**		10	0	Very low	Low	High	Very high
	Plant uptake (crop yield)**		5	0	Very high	High	Low	Very low
	Management practice		10	15	Best	Good	Average	Worst

Fig. 5.1: Factors influencing the leaching-runoff potential of nitrogen (Franke et al., 2013).

Figure 5.1 shows the information to make the original Tier 1 calculation from Franke et al. (2013). The table categorizes influencing factors and assigns a score, ranging from very low (0) to very high (1). Each factor is assigned a weight, indicating its relative importance in the overall assessment.

Python script

Table 5.1 helps to process the information taken from the HWSD 2.0 viewer to the Python script for the automated Tier 1 method. In the HWSD 2.0 viewer, users can select one of 13 soil types, ranging from heavy clay to sand, and one of 7 drainage classes, from Very Poorly Drained (VP) to Excessively Drained (E). The soil type number and drainage class abbreviation serve as inputs for the automated Tier 1 method.

Tab. 5.1: List of soil types and drainage classes with their respective descriptions (HWSD, 2024).

Soil type	Description	Drainage class	Description
1	Clay (heavy)	VP	Very poorly drained
2	Silty clay	P	Poorly drained
3	Clay (light)	I	Imperfectly drained
4	Silty clay loam	MW	Moderately well drained
5	Clay loam	W	Well drained
6	Silt	SE	Somewhat excessively drained
7	Silt loam	E	Excessively drained
8	Sandy clay		
9	Loam		
10	Sandy clay loam		
11	Sandy loam		
12	Loamy sand		
13	Sand		

Optimization

Table 5.2 presents the weight sets that is used in the optimization of the Tier 1 method. Each row represents a different weighting scenario, where the relative importance of influencing factors is adjusted to accommodate an increase in the application rate weight. To streamline the optimization process, ten predefined weight sets were created, with the application rate weight increasing in increments of 5%, starting from the original 10% and reaching up to 55%.

Tab. 5.2: Possible weight sets for optimization

	N-dep	Tex_l	Tex_r	Drain_l	Drain_r	Precip	N-fix	**App**	Uptake	Prac
1.	10%	15%	10%	10%	5%	15%	10%	**10%**	5%	10%
2.	10%	10%	10%	10%	5%	15%	10%	**15%**	5%	10%
3.	10%	10%	10%	10%	5%	10%	10%	**20%**	5%	10%
4.	10%	10%	10%	10%	5%	10%	5%	**25%**	5%	10%
5.	5%	10%	10%	10%	5%	10%	5%	**30%**	5%	10%
6.	5%	10%	5%	10%	5%	10%	5%	**35%**	5%	10%
7.	5%	10%	5%	5%	5%	10%	5%	**40%**	5%	10%
8.	5%	5%	5%	5%	5%	10%	5%	**45%**	5%	10%
9.	5%	5%	5%	5%	5%	10%	5%	**50%**	5%	5%
10.	5%	5%	5%	5%	5%	5%	5%	**55%**	5%	5%