

Increasing Nutrient Circularity and Reducing Water Pollution Through Anaerobic Digesters

by

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Author's Declaration

This thesis consists of material all of which I authored or co-authored: see Statement of Contributions included in the thesis. This is a true copy of the thesis, including any required final revisions, as accepted by my examiners.

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Statement of Contributions

I would like to acknowledge my co-authors Dr. Nandita Basu and Dr. Juliane Mai who contributed to the research described in this thesis.

Abstract

While the intensification of agricultural practices over the last few decades has increased livestock and crop production, it has also led to unintended environmental consequences such as harmful algal blooms, drinking water contamination, and increased emissions of greenhouse gasses. Much of the increase in crop and livestock production can be attributed to a shift towards specialized agriculture which has resulted in the decoupling and spatial separation of livestock and crop systems. The spatial separation of the two systems has disrupted the circular flow of nutrients in agricultural systems. Relinking the livestock-nutrient economy has been identified as a strategy to reduce the overall environmental burden of the sector. The use of anaerobic digesters to manage livestock manure presents a promising pathway towards the recoupling of crop and livestock systems.

Anaerobic digesters, or also referred to as biodigesters, utilize anaerobic decomposition to transform organic wastes into valuable by-products. During the digestion process, methane – a potent greenhouse gas emitted in traditional manure management – is captured to produce biogas which is a source of renewable energy. The process also produces digestate which is a nutrient rich effluent that can be applied to cropland as a fertilizer source. The nutrient dense nature of digestate, and the potential revenue from biogas production enable it to be economically transported over a greater distance than untreated manure – thereby providing a pathway to enhance the nutrient circularity in spatially separated livestock and crop systems. However, there is concern that digestate use can result in greater nitrogen leaching losses than manure.

The work presented in this thesis estimates the nitrogen leaching losses from the corn and soybean cropland across 263 regions in Ontario and assesses the water quantity implications of manure and digestate land-application. To do this, a DeNitrification-DeComposition (DNDC) model was developed for each region. The models were calibrated individually to observed crop yields from 2011 and 2021. The calibrated models were able to capture the general magnitude and annual variation in reported corn and soybean yields across the study region. The median error between simulated and observed crop yields across all regions was 5.8% (mean absolute percent error). Corn crops were provided with synthetic fertilizer at an optimal rate, as determined by calibration. The results of the calibration showed that observed crop yields across the study region could be met through the application of 69% of the nitrogen fertilizer purchased in Ontario

in 2021. This finding suggests corn nitrogen requirements are met through the application of purchased synthetic fertilizer while manure is applied to cropland in addition of crop needs. Next, I used livestock population data to estimate the quantity of manure nitrogen produced in each region. Using the calibrated DNDC models, I simulated a number of scenarios which explored various manure and digestate distribution configurations across the landscape.

The results of this work show that when digestate was substituted for manure and subject to the same transportation constraints, the amount of nitrogen lost by leaching across the study region increased by 6% (from 46.77 to 49.42 $kt\ N\ yr^{-1}$). However, when the digestate distribution configuration was altered to reflect re-distribution from a centralized biodigester and its ability to be transported over a greater distance, the amount of nitrogen lost through leaching across the study region was reduced by 7% (43.42 $kt\ N\ yr^{-1}$). These findings show that when digestate was used as a direct substitute for manure and applied at equal rates based on total nitrogen content, it contributed to increased nitrogen leaching losses. However, when the distribution of the digestate was considered at a regional scale and the system dynamics of the biodigester were accounted for, the use of digestate reduced the total nitrogen leaching losses across the study region. This research shows that biodigesters can provide benefit to water quality when considered at a regional scale.

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Chapter 1 – Introduction

1.1 The Environmental Impacts of the Agriculture Sector

To meet the needs of a growing world the agricultural sector has undergone continuous advancements and transformations to increase outputs. However, the intensification of agricultural practices over the last five decades has resulted in widespread air and water pollution. The agricultural sector, and associated land use changes, was estimated to contribute 22% – or 13 billion tonnes carbon dioxide equivalent ($CO_2 eq$) – of global anthropogenic greenhouse gas (GHG) emissions in 2019 (IPCC Working Group, 2022). Agriculture is also the largest contributor of nutrients, such as nitrogen and phosphorus, to surface waters globally (Beusen et al., 2016); causing harmful algae blooms and the eutrophication of surface water systems (Tamminga, 2003; Vu et al., 2020). Nutrient pollution from agriculture can also lead to nitrate contamination of groundwater systems which poses a severe threat to human health (M. H. Ward et al., 2018). Livestock manure plays a large role in the agricultural sector's overall environmental impact.

The storage and handling of livestock manure is estimated to contribute between 3 (IPCC Working Group, 2022) and 10% (Owen & Silver, 2015) of global GHG emissions from agriculture; with a growing body of research suggesting the emissions from livestock manure are greatly underestimated by current accounting techniques (VanderZaag et al., 2013; N. Ward et al., 2024). Agricultural operations typically store manure throughout the year and apply it to cropland in the spring; replenishing the soil's nutrient supply before crops are sown. Manure is stockpiled and strategically applied to cropped land to align with current recommendations for agricultural best management practices (Ministry of Agriculture, Food and Rural Affairs, 2024) and Fertilizer Canada's 4R's Nutrient Stewardship Program (*4R's Across Canada*, 2019), among other programs aimed at lessening the water quality impact of agricultural practices. While applying manure to cropped land at the right time can reduce nutrient losses and thereby benefit water quality, manure begins to decompose while stored which emits harmful GHGs. Commonly used manure storage systems (i.e. piles and tanks) store manure under anaerobic conditions – or without sufficient oxygen supply. When manure decomposes in an anaerobic state it produces large amounts of methane (CH_4) – a GHG with almost 30 times the global warming potential of CO_2 (EPA, 2024). In recent years there has been an increase in the amount of manure stored in

anaerobic conditions which has resulted in an increase in manure related emissions (Niles & Wiltshire, 2019; Wightman & Woodbury, 2016). Under current practices, manure continues to produce harmful GHGs and contribute to climate change. As livestock populations increase, improvements to manure management practices are essential.

Livestock manure was estimated to contribute 7.8 of the 56 million tonnes of $CO_2\ eq$ emitted by the Canadian agricultural sector in 2022 (Environment and Climate Change Canada, 2023). While air and water pollution from livestock manure are a concern across Canada, Ontario is a Canadian province where the entanglements of agricultural activities and water quality decline are on full display. The province of Ontario is an economic and agricultural center in Canada. It is home to almost 40% of Canada's population (Statistics Canada, 2024a) and 25.5% of the country's agricultural operations (Government of Canada & Canada, 2022). The Great Lakes – which are estimated to make up approximately one fifth of the world's freshwater – border the province and provide drinking water to an estimated 80% of the population (Government of Ontario, 2023). The Great Lakes also support the province's abundant and diverse agricultural sector. However, the lakes face a water quality crisis; evident by the severe algae blooms which appear in increasing frequency on the surface of Lake Erie – the shallowest Great Lake (NCCOS, 2019). Algae blooms have widespread impacts. They impact economies, fisheries, cultural practices, and recreational activities which depend on the health of a lake. In 2014, over half a million people lost access to drinking water due to a harmful algae bloom in Lake Erie (Brooks et al., 2016). The algal blooms are caused by an overabundance of nutrients deposited in the lake – a process which has been linked to the increasing agricultural presence in the watershed (Michalak et al., 2013). Widespread improvements to agriculture nutrient management in Ontario are necessary to preserve the health of the Great Lakes and reduce the overall impact of the Canadian agricultural sector.

1.2 Improving Agricultural Nutrient Circularity

Improvements to nutrient circularity have long been identified as a pathway to mitigate the negative environmental impacts of the agricultural sector (Harder et al., 2021; van der Wiel et al., 2019). Nutrient circularity involves the use of livestock manure to supplement agricultural soils with the nutrients necessary to sustain crop production (i.e. Nitrogen, Phosphorus, Potassium). This is in opposition to a linear nutrient economy, where commercial (also referred to as synthetic) fertilizer is used to meet crop nutrient demands. The production of synthetic fertilizers is a very

energy intensive process that has a large environmental impact. The production and use of synthetic nitrogen fertilizers was estimated to produce 1.13 billion tonnes of CO_2 eq, globally, with production and application accounting for 39% and 59%, respectively (Menegat et al., 2022). The use of manure to meet crop nutrient demands, in place of synthetic fertilizer, provides both energy savings (Ceotto, 2005; Wiens et al., 2008) and benefits to soil health (EPA, 2018). However, while much of crop nutrient demand can be satisfied by the reuse of manure (Akram et al., 2019b; Metson et al., 2016) there are economic and logistical constraints associated with it (Akram et al., 2019b).

There has been a shift towards specialized agriculture – a process where farm revenue is generated through the production of a single product (Statistics Canada, 2016). This has led to the decoupling and spatial separation of livestock and crop systems (Akram et al., 2019a; Flynn et al., 2023). With the separation of livestock and crop systems on the landscape, manure has become concentrated in regions with large livestock populations – termed manure hotspots (Spiegel et al., 2020). Conversely, there has been a development of regions with an abundance of crops, and thereby large nutrient requirements. While manure can theoretically be transported from manure hotspots to regions with large nutrient requirements, there is a lack of structures in place to facilitate this redistribution (Spiegel et al., 2020). A manureshed is a term used to describe the sharing of manure from regions with excess manure to regions with high nutrient demand irrespective of human boundaries (Spiegel et al., 2020). The concept has been introduced as a solution to combat the uneven spatial distribution of manure across the landscape. However, manure redistribution relies on the voluntary collaboration of a number of stakeholders which poses unique social and logistic challenges (Meredith et al., 2022). It also requires the transportation of manure which is often hindered by economic constraints.

Manure transportation is a very expensive process. Cost often limits the distance over which manure is moved, rather than environmental or logistical constraints (Ceotto, 2005; Cobo et al., 2019). As a result of this, manure is typically not transported further than 10 kilometers from where it was produced (Schnorf et al., 2021). For crop operations without access to manure, it is often more economical to use synthetic fertilizer than to transport manure. A study conducted in 2019 found that to redistribute manure from regions with a surplus supply to deficient regions in Sweden would cost almost 4 times more than the cost of purchasing an equivalent amount of nutrients in

the form of synthetic fertilizer (Akram et al., 2019b). This is partly due to the volume of manure that would need to be transported. Processes which increase the nutrient density of manure (i.e. pelletizing or drying processes) can lower the costs associated with its transport (Meredith et al., 2022). Additionally, technologies which utilize manure to generate revenue (i.e. renewable energy production) can aid in offsetting transportation costs and thereby extend the distance that manure can be cost effectively transported (Meredith et al., 2022). A promising pathway towards enhancing the nutrient circularity in the agricultural sector is the integration of anaerobic digesters into current manure management practices.

1.3 Biodigesters as a Tool to Enhance Nutrient Circularity

Anaerobic digesters, also referred to as biodigesters, are an advantageous agricultural waste management system because they break down a wide variety of organic waste (i.e. manure, wastewater sludge, food waste) to produce renewable energy while enhancing the circularity of agricultural operations by conserving nutrients during digestion (Cortez et al., 2022). Biodigesters are contained systems which facilitate the anaerobic decomposition of organic wastes. In 2023, there were over 30 agricultural anaerobic digestion operations in the province of Ontario (Canadian Biogas Association, 2023b). The adoption of agricultural digesters is growing in popularity with the number of operations in Ontario increasing annually. Wastes fed to a biodigester, known as feedstocks. Livestock manure is the most common feedstock for biodigesters due to the abundance of livestock globally (Sudalyandi & Jeyakumar, n.d.).

When organic matter is broken down in anaerobic conditions methane and carbon dioxide are produced. When anaerobic decomposition occurs in a biodigester, rather than in an open manure pile or storage tank, the methane and carbon dioxide are captured by the digester. This process prevents the harmful GHGs from being released to the environment. The EPA estimates that if American hog and dairy operations utilized biodigesters to manage manure they could reduce their methane emissions by up to 85% (EPA, 2018). In addition to GHG reduction, biodigesters offer a number of benefits when used as a manure management system such as reduced odors (Orzi et al., 2015), decreased volume of manure (Möller et al., 2010), and the elimination of some pathogens (Orzi et al., 2015; Rajagopal et al., 2019). However, much of the benefit of a biodigester system lies in its by-products: biogas and digestate.

The methane and carbon dioxide produced during anaerobic digestion are collected by the biodigester and referred to as biogas. Biogas can be harnessed and utilized as an energy source thereby offsetting more environmentally taxing forms of energy production, such as fossil fuels (Canadian Biogas Association, 2023a). In addition to offsetting fossil fuel production, there is an economic incentive to biogas generation due to its market value (Canada Revenue Agency, 2010). In Canada, approximately 50% of utilized biogas is used for electricity, 22% for heating, and the remaining 28% is used as renewable natural gas (Canadian Biogas Association, 2023b). The organic material that is not transformed to biogas leaves the digester as a nutrient rich effluent known as digestate. As the nitrogen and phosphorus content of the manure feedstock are preserved throughout the anaerobic digestion process, digestates are considered to have good fertilization potential (Möller & Müller, 2012; Sharifi et al., 2019; Tambone et al., 2010). Therefore, they can be applied to cropland to supplement crop nutrient requirements and have been found to work as well as synthetic fertilizers or manures (Rossi et al., 2023; Sogn et al., 2018; Tambone et al., 2010). The reuse of digestates on cropland presents a viable pathway to recoup livestock and crop systems because digestates can be transported over a longer distance than manures.

The enhanced transportation distance of digestate is due to two key aspects of the biodigester system. During the anaerobic digestion process, feedstock volume is reduced (Möller & Müller, 2012). However, as nitrogen and phosphorus content of the feedstock is conserved, digestates possess a higher nutrient density than their manure feedstocks. In addition, the revenue generated from the production of biogas can theoretically be used to offset the cost of digestate transportation. Together, the increased nutrient density of digestate and the revenue generated from biogas production improve the economics of transportation. The maximum distance that digestate can be transported varies based on the objectives of the biogas plant.

The maximum distance over which digestate can be optimally transported is referred to as break even distance and it can be derived based on environmental, economic, or policy constraints. For instance, guidelines in Italy require the emissions from biogas plants to be at least 35% lower than those of fossil fuel production (Capponi et al., 2012). Capponi et al. (2012) found that the break-even distance of digestate transportation, based on the Italian guidelines, was approximately 192 km. However, the objectives of a biogas plant could also be to maximize revenue irrespective of emissions. This would of course result in a lower digestate breakeven

distance in order to reduce transportation expenses. When the digestate breakeven distance is based on economic constraints, a number of factors such as plant size, revenue, feedstock, and feedstock cost play a role in its calculation (Yazan et al., 2018). While digestate have a high fertilization value, there are some environmental concerns surrounding the nitrogen losses associated with its use.

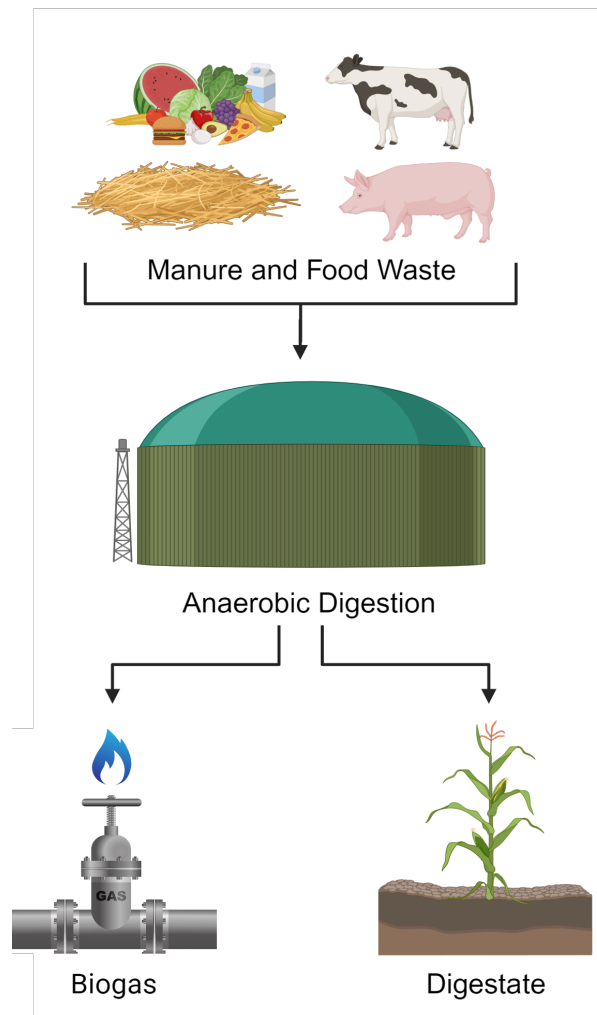


Figure 1: Biodigester system. Created with BioRender.com.

1.4 Environmental Concerns for Digestate Land-Application

There are environmental concerns that the land-application of digestates may lead to greater nitrogen losses compared to untreated manure. There are two commonly cited nitrogen loss concerns: 1) the potential for increased nitrogen gaseous emissions, discussed in Section 1.4.1

and 2) increased nitrogen leaching rates, discussed in Section 1.4.2. The work presented in this thesis explores the latter.

1.4.1 Increased Gaseous Emissions

When nitrogen is applied to cropland to supplement crop nutrient requirements a portion of it is lost through gaseous emissions. Due to its high inorganic nitrogen content and elevated pH, digestate is especially susceptible to nitrogen losses through ammonia volatilization (Nicholson et al., 2017). While gaseous nitrogen losses can occur at any point in the digestate life cycle, they predominantly occur during storage and land-application (Möller & Müller, 2012; Y. Zhang et al., 2021).

A number of field-based studies have explored the gaseous nitrogen emissions which occur as a result of digestate application. Some studies have reported that the land-application of digestate produces more nitrogen emissions compared to untreated manure (Evans et al., 2018; Nicholson et al., 2017; Y. Zhang et al., 2021). A study conducted in 2018 utilized wind tunnels to quantify the ammonia emissions from digestate and liquid manure application (Evans et al., 2018). The study found, when applied at the same rate based on total nitrogen content, the digestate exhibited significantly larger ammonia emissions, however, when the emissions were normalized by the total ammonium, the emissions were similar. The gaseous emissions produced during application reduce the nitrogen available for the crops.

Large gaseous emissions from digestate application can reduce its fertilization potential. A 2021 study compared the emissions from digestate and pig manure (Y. Zhang et al., 2021). The authors reported that even though the digestate had more available nitrogen than the pig manure, the application of the digestate produced enough gaseous nitrogen losses to offset its enhanced nitrogen availability (Y. Zhang et al., 2021). When applying digestates, the amount of nitrogen lost through gaseous emissions can range anywhere from 10% (Möller et al., 2010) to 40% of the total nitrogen content (Nicholson et al., 2017). However, some studies have reported that digestates emit less nitrous oxide during application than manure (Baral et al., 2017; Schwager et al., 2016) or compost (Posmanik et al., 2023). The lower nitrous oxide emission may be due to the reduced volatile solid content of digestates (Baral et al., 2017).

1.4.2 Increased Leaching Losses

There are also concerns that the nitrogen leaching potential of digestates may be greater than those of manures or synthetic fertilizers due to the changes to the nitrogen profile that occur during anaerobic digestion. A number of field and pot studies have been conducted to explore this concern, yet there is heterogeneity in published results.

Manure based digestates have been found to contribute to greater nitrogen leaching losses, compared to untreated manures, at the field scale (Nicholson et al., 2017; Schwager et al., 2016) and pot scale (Pranckietienė et al., 2023). However, contrary results have also been reported. Some studies have found that the nitrogen leaching potential of manure based digestates are similar to those of untreated manures when applied at the similar rates (Pranckietiene et al., 2023; Svoboda et al., 2013). Similarly, a 2017 field study showed comparable nitrogen leaching rates between field treatments of food-based digestate and untreated animal slurry (Nicholson et al., 2017). In some cases when compared to synthetic fertilizers, digestates have been found to cause lower nitrogen leaching rates (Rossi et al., 2023; Tshikalange et al., 2020).

1.4.3 Understanding the Spatial Variation of The Impacts

While there are environmental opportunities and challenges associated with the application of digestate on cropland, the magnitude of both varies spatially – as evident by the heterogeneity in published field scale results. A number of factors can influence the nitrogen leaching potential of digestate such as soil texture, application method, topography, and precipitation (Nkoa, 2014). This was shown in a pot experiment conducted in 2018, where the nitrogen leaching rates displayed by digestate and raw manure treatments were found to be similar to those of a synthetic fertilizer when applied in a loam soil (Sogn et al., 2018). However, when the same treatments were applied to a sandy soil, the digestate and manure treatments displayed lower nitrogen leaching rates than the synthetic fertilizer. The emissions from digestate application also vary based on several factors. A 2020 study found that the magnitude of methane emissions that occurred after digestate application was dependent on the soil type, while the magnitudes of nitrous oxide and carbon dioxide emissions were a function of how the soil was managed in previous growing seasons (Rosace et al., 2020).

Most studies which examine the impacts that stem from the land-application of digestate are field scale experiments. However, at the field scale the spatial variation in impacts cannot be assessed and it is difficult to capture the benefits and tradeoffs that a biodigester can pose at the system scale. In this thesis, a regional modeling approach is taken to account for the impact that spatially varying factors, such as climate and soil conditions, have on the nitrogen leaching losses of digestate.

1.5 Modeling Nitrogen Losses in Agroecosystems

Modeling techniques can be employed to investigate the environmental impacts of various agricultural management practices before they are implemented. There are a number of process-based models that simulate the biogeochemical processes which occur in agroecosystems. In 2018, a study was conducted to compare the water simulations of three agroecosystem models: DNDCv.CAN – a Canadian offshoot of the DeNitrification-DeComposition (DNDC model) –, Holos, and the Versatile Soil Moisture Budget (VSMB) model (Guest et al., 2018). The performance of each model to estimate evapotranspiration, soil moisture, runoff, and drainage was evaluated. The results of the study showed that overall DNDCv.CAN performed the best at a daily timescale and at a monthly timescale. The authors suggest one reason DNDCv.CAN outperformed the other models was due to its consideration of daily crop growth, nitrogen movement, and climate stresses when determining the water budget.

In 2020 DNDCv.CAN's ability to simulate nitrogen losses to runoff and tile drains was compared with that of the Root Zone Water Quality Model (RZWQM2) (Smith et al., 2020, 2019). The RZWQM2 model provides similar functionality to the DNDCv.CAN model however it uses complex equations to simulate biogeochemical processes and thus requires increased computational capacity to operate. Smith et al. (2020) found that DNDCv.CAN displayed similar ability to estimate nitrogen losses to runoff and leaching losses to tile drains as the RZWQM2 model, across the tested sites. Due to its shown success in simulating water and nitrogen movements in agroecosystems, the DNDCv.CAN model was used in this thesis.

1.6 The DNDC Model

The DNDC model is a widely used carbon and nitrogen process-based model and was originally developed to simulate nitrous oxide emissions (Li et al., 1992). Since its development, the model

has continued to evolve, resulting in a model with capacities to estimate crop yields, carbon sequestration, nitrogen runoff and leaching losses, as well as carbon and nitrogen gaseous emissions in agroecosystems (Institute for the Study of Earth, Oceans and Space, 2012). To model the carbon and nitrogen cycling that occur within agricultural soil, DNDC simulates a number of biogeochemical processes including decomposition, nitrification, denitrification, ammonia volatilization, and fermentation, among others (Institute for the Study of Earth, Oceans and Space, 2017).

Over the past two decades, many versions of DNDC have been developed to better suit specific climates (Gillespie et al., 2014). A Canadian version of the model (DNDCv.CAN) was developed to better account for the influence of a colder climate (Kröbel et al., 2011; Smith et al., 2013). Since its creation, the sub-models of DNDCv.CAN have undergone numerous improvements to better tailor the model to simulate crop growth (Kröbel et al., 2011; Smith et al., 2013), evapotranspiration (B. Dutta et al., 2016), soil temperature (Baishali Dutta et al., 2018), as well as tile drainage and soil hydrologic processes (Smith et al., 2020) within a Canadian climate. The DNDCv.CAN model has shown success in its ability to simulate nitrogen losses via nitrous oxide emissions (Uzoma et al., 2015), ammonia volatilization (Congreves, Grant, et al., 2016), nitrate leaching (J. Zhang et al., 2021), and plant uptake (J. Zhang et al., 2021) making it an ideal candidate for exploration of the nitrogen losses associated with agroecosystems. In this thesis, I use the DNDCv.CAN model (Version 9.5.8) to explore the nitrogen leaching which occurs as a result of various manure and digestate distribution configurations in Ontario. Henceforth, DNDC and DNDCv.CAN are used interchangeably to refer to the Canadian version of the DNDC model.

1.7 Objectives

The overall objective of this work is to quantify agriculture-related nitrogen leaching losses across Ontario and evaluate the role of an anaerobic biodigester to mitigate these losses. To achieve this, I will 1) adapt the DNDC model to simulate crop yields across 263 regions in Ontario and 2) use the regional DNDC models to explore the nitrogen leaching losses associated with the land-application of anaerobic digestate and untreated manure under multiple nitrogen application scenarios.

Chapter 2 - Background

The results of a literature review are presented in Chapter 2 to provide background context for the work presented in this thesis. Nitrogen losses in agroecosystems and their environmental impacts are discussed in Section 2.1. An exploration into the physical and chemical properties of digestate is presented in Section 2.2. Finally, the DNDC model framework is outlined in Section 2.2.

2.1 Nitrogen and the Environment

2.1.1 *The Nitrogen Cycle*

Nitrogen takes many forms, and the processes of the nitrogen cycle facilitate the conversion between them. These transformational processes are important as many organisms can only utilize select forms of nitrogen. The most abundant type of nitrogen is nitrogen gas (N_2) (Bernhard, 2010; Robertson & Groffman, 2024). The process of nitrogen fixation – performed either by nitrogen fixing bacteria, lightning, or industrial practices – breaks apart inorganic N_2 molecules to create inorganic ammonia (NH_3). When these processes occur in soil, the ammonia produced is dissolved in soil water and is converted to ammonium (NH_4). The process of nitrification transforms ammonium intermediately to nitrite (NO_2^-), and then to nitrate (NO_3^-). Both nitrite and nitrate are inorganic forms of nitrogen. Conversely, denitrification converts the products of nitrification back to atmospheric nitrogen gas.

The waste products of living organisms are largely composed of organic nitrogen, which comes in many forms (Bernhard, 2010; Robertson & Groffman, 2024). The process of mineralization breaks down organic nitrogen to inorganic ammonia (or ammonium in soils). The process of immobilization reverses the process of mineralization and transforms ammonium back into organic nitrogen. Nitrogen is continually changing forms, and the quantity of nitrogen existing in any one form is dependent on the rates of the aforementioned processes.

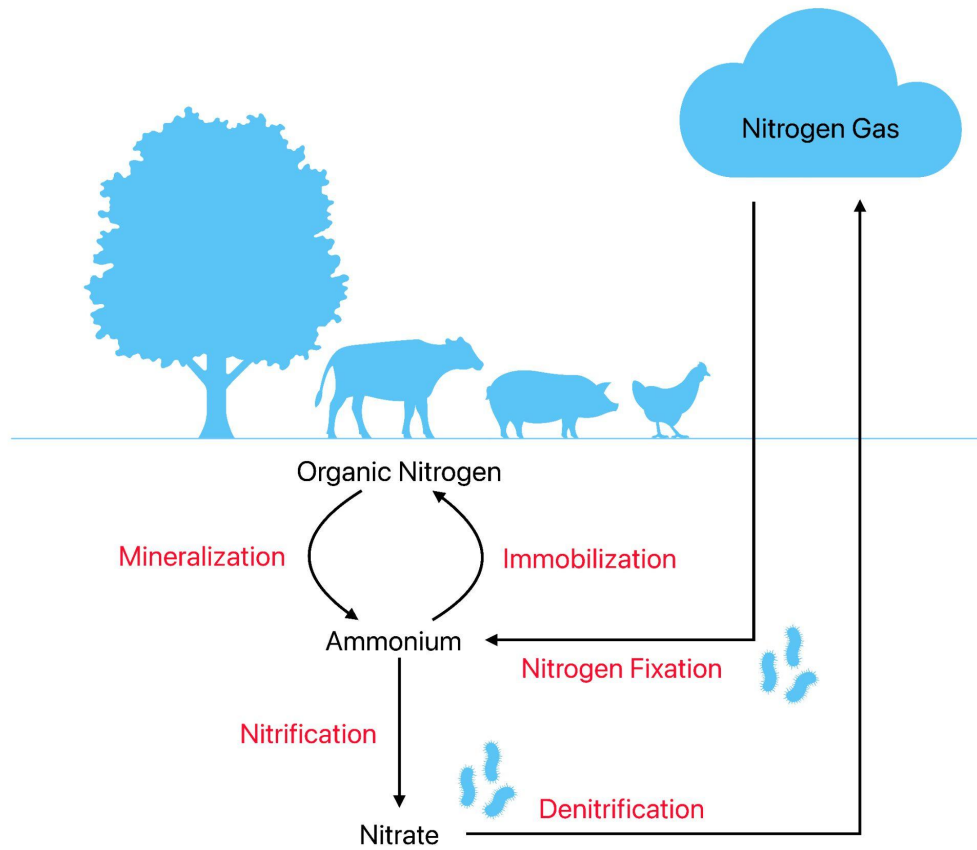


Figure 2: Simplified nitrogen cycle.

2.1.2 Plant Available Nitrogen

Plant available nitrogen (PAN) is a term used to describe nitrogen present in a form that is accessible to plants. Plants can only access inorganic nitrogen. More specifically, the two forms of PAN are NO_3^- and NH_4^+ (Robertson & Groffman, 2024). However, the majority of nitrogen present in livestock manure exists in organic form. Yet, manure can still act as a source of nitrogen for plants due to the processes of the nitrogen cycle. Mineralization transforms unusable nitrogen into PAN, and conversely, immobilization converts PAN to unusable nitrogen. When organic fertilizers are applied to cropped land, the rate at which the plants can access the nitrogen in the manure is governed by the rates of mineralization and immobilization in the soil.

On the other hand, synthetic fertilizers are often made, in full or in part, from inorganic nitrogen. When applied to cropped land, plants can readily access all of the nitrogen contained in the

fertilizer without relying on mineralization to make the nitrogen accessible. This creates complexity when replacing organic fertilizers with inorganic fertilizers, as it is not a one-to-one replacement. When using organic fertilizers, such as manure or digestate, the PAN – or inorganic nitrogen – content of each fertilizer must be considered alongside soil mineralization rates.

2.1.3 Nitrogen Losses in Agroecosystems

When nitrogen is applied to cropland a portion of the nitrogen is inevitably lost from the system. Nitrogen losses in agroecosystems are a tri-fold problem. When nitrogen is lost from cropped land, the amount available for crops is reduced. This can cause nitrogen stress in crops resulting in lower crop yields. Farmers may estimate the predicted losses on their land and account for them by applying additional nitrogen. However, the application of additional nitrogen can increase farm operating costs. Nitrogen lost from agroecosystems also has negative environmental impacts. Agricultural nitrogen losses occur through three main pathways: leaching, runoff, and gaseous emissions.

Nitrate (NO_3^-) is a water soluble form of nitrogen which allows it to be mobilized by water movement in the soil profile (Killpack & Buchholz, 2022a). Water travels downward through the soil profile at a rate governed by the soil's hydraulic conductivity until it reaches the water table. As the water moves through the soil profile it carries nitrate molecules with it, depositing the nitrate in groundwater reserves. Nitrate contamination is a large concern as groundwater is a common source of drinking water (EPA, 2013). It is estimated that groundwater supplies over 20% of Ontario's population with drinking water (Simpson & Myslik, 2021). When groundwater is contaminated with nitrate it can cause adverse health impacts, especially in infants (M. H. Ward et al., 2018).

When water is applied to the soil surface at a rate greater than the soil's hydraulic conductivity, or at an amount greater than the soil can hold, the water will no longer infiltrate down the soil column but rather travel along the soil surface as runoff. As with the process of leaching, when runoff travels along the soil surface it carries nitrate molecules on the soil surface along with it. Runoff leaves the boundaries of agroecosystems and joins nearby water courses. When the nitrate rich runoff is deposited in a water course it can have devastating water quality impacts

such as eutrophication (Tamminga, 2003). In addition to losses to water sources, nitrogen can also be lost from agroecosystems via gaseous emissions.

While ammonium is an essential form of nitrogen to sustain plant life, it is susceptible to nitrogen losses through volatilization (IPNI, n.d.). When nitrogen fertilizers are applied to soil surfaces, ammonium is easily transformed to ammonia gas. The rate at which ammonium is lost through volatilization is dependent on the pH of the fertilizer, the method of application, soil condition, and climate. Elevated pH levels, temperature, soil moisture content, and wind speed all increase the rate of volatilization. Fertilizer application methods that limit the time fertilizers spend on the soil surface (i.e. injection or incorporation) can greatly reduce gaseous nitrogen losses. While denitrification principally works to convert nitrite and nitrate to harmless nitrogen gas, it also creates intermediate gaseous products – nitric oxide (NO) and nitrous oxide (N_2O) – that can be lost from the system and have negative environmental impacts (Bernhard, 2010). Denitrification is carried out by soil microorganisms and so the organic matter content of a soil will influence its rates of denitrification (Killpack & Buchholz, 2022b). Denitrification occurs under anaerobic conditions and therefore occurs more rapidly in wet soils. Minimizing nitrogen losses in an agroecosystem, through all pathways, can help to ensure crop nitrogen requirements are met as well as reduce the water quality and climate change contributions of the sector.

2.2 Digestate Characteristics

The properties of digestate influence how it will interact with soil, water, and crops once land applied. However, the chemical and physical properties of digestate are difficult to define, as they vary based on a number of factors (EPA, 2020; Fuchs & Drosch, 2013; Möller et al., 2010). In general, some assumptions can be made. When compared to untreated manure, digestates tend to contain more ammonia, a lower carbon nitrogen ratio, less carbon, a lower biological oxygen demand, reduced viscosity, and a higher pH (Möller & Müller, 2012). A review study conducted in 2012 defined the general range observed for various digestate properties, displayed in Table 1, further illustrating the diverse range of properties digestate can encompass (Möller & Müller, 2012).

Table 1: Average properties of digestate. Data from Moller & Muller (2012)

Property	Range (%)
Dry Matter	1.5 - 13.2
Total N	3.1 - 14.0
Total P	0.6 - 1.7
Total K	1.9 - 4.3

During its lifecycle, the properties of digestate are altered many times. Feedstock is transformed during the anaerobic digestion process to become digestate. Similarly, digestate undergoes multiple transformations from the time it leaves the biodigester to the time it is land-applied. Each transformation alters the properties of the digestate and influences how it will interact with the soil, water, and crops once land applied. This series of transformations makes it hard to generalize the properties of digestate in its final form. While tracking the transformations that occur during each process is possible for a given site, each biodigester operation is unique and can include various post-digestion processes depending on the desired goals of the operation, adding a degree of difficulty to generalizing digestate properties. However, the most prevalent transformational processes include feedstock selection, digestion processes, and solid liquid separation.

2.2.1 The Influence of Feedstock Selection

The feedstock used to fuel the anaerobic digester, has a large influence on the final properties of the digestate and the amount of biogas produced. Multiple feedstock types can be fed to the digester simultaneously, in a process known as co-digestion. Co-digestion serves many purposes but is foremost utilized to increase biogas production (EPA, 2020). When considering feedstocks for co-digestion, additional attention must be given to ensure the feedstocks are compatible in a way that will increase biogas production without impeding the performance of digester.

In 2017, Risberg et al. noted the heterogeneity in published literature regarding the impacts of digestate application on soil health and hypothesized it was due to variation in properties of the digestates used between studies. To explore this, they analyzed the properties of 20 digestates

made from various feedstocks. Select results of this study are summarized in Table 2 to show the large influence feedstock selection plays in determining the properties of the digestate produced.

Table 2: Properties of digestate based on feedstock selection. Data from Risberg et al. (2017).

Feedstock Type	Dry Matter	Total Carbon	Total Nitrogen	NH4 Nitrogen	Organic Nitrogen
	%	kg/ton			
100% cow manure	7.4	34	3.4	2.2	1.2
99% cow manure, 1% fodder and silage waste	6.1	26	4.1	2.8	1.3
75% manure, 25% food waste	3.9	15	4.8	3.6	1.2
75% household organic waste, 25% manure	1.1	4.3	2.6	2.1	0.5
80% cow manure, 20% household organic waste	4.1	16	5.7	4.2	1.5
90% cow manure, 5% food processing industry waste	4.3	16.9	3.5	2.4	1.1

Feedstock selection also plays a role in the stability of the digestate. The stability of a digestate describes its resistance to mineralization and it dictates if the digestate can be directly land-applied or if it requires further processing (Alburquerque et al., 2012). Unstable digestates lead to a large amount of nitrogen immobilization which reduces the fertilization value of the digestate. Digestate stability is largely dependent on feedstock type and thus the feedstock selection process should also consider stability (Alburquerque et al., 2012).

2.2.2 *Property Alteration During Anaerobic Digestion*

When feedstock enters the anaerobic digester its physical properties and nutrient profile are altered by the digestion process. The digestion process reduces the volume of the feedstock (Möller & Müller, 2012). The volume reduction that occurs during the transformation from feedstock to digestate largely depends on the type of feedstock used. Feedstocks such as cereal grains are highly degradable, and therefore will experience a greater volume reduction (Möller &

Müller, 2012). A study conducted in 2010 explored the volume reduction of two biogas plants which utilized various crop residues as feedstock (Möller et al., 2010). The authors found that the fresh matter volume reduction of the feedstock was between 25-30%, on average. The reduction in feedstock volume comes from a reduction in dry matter content. The water content of the feedstock is preserved throughout digestion. The degree of feedstock decomposition is also governed by the type of anaerobic digestion used.

There are three major types of anaerobic digestion: psychrophilic, mesophilic, and thermophilic (EPA 2020). Psychrophilic digestion occurs at temperatures less than 20 °C, mesophilic digestion operates from 30 °C to 40 °C, and thermophilic digestion occurs at temperatures from 50 °C to 65 °C. The operating temperature determines the speed at which the organic material breaks down and the retention time of the digester. Retention time refers to the time the feedstock remains in the digester and is typically determined based on the length of time required to sufficiently digest the organic matter while maximizing biogas yield (EPA, 2020). The temperature that the anaerobic digester operates at determines the speed at which the feedstock breaks down and also determines the amount of biogas generated. The higher the temperature of the digester, the quicker organic matter will be broken down and the lower the required retention time. Increasing the retention time can have a positive impact on the by-products of anaerobic digestion, such as increased biogas yield and increased stability of digestate but has a negative impact on operational costs. The nitrogen profile of the feedstock also undergoes transformation. Most of the feedstock's organic nitrogen content is converted to inorganic ammonium (Czekala, 2022; Möller et al., 2010; Risberg et al., 2017).

2.2.3 Solid-Liquid Separation

There are a multitude of treatments that can be applied to digestate once it leaves the biodigester. Treatments are typically applied to alter the properties of digestate to align with the goals of the biogas plant, therefore post-digestate treatment processes vary by operation. However, the most common post-digestion treatment is solid-liquid separation. Solid-liquid separation is a common treatment used to increase the ease of digestate handling and it is a common predecessor to most other post-digestion treatment methods. The high-water content of digestate can make transportation, storage, and land application of digestate difficult (Valentinuzzi et al., 2020). Solid-liquid separation results in a solid portion with a higher dry matter content than the feedstock. The

solid portion can be stored in piles and land applied using standard manure spreading techniques and equipment (Lyons et al., 2021). The liquid portion can be transported by tankers, and land-applied using liquid fertilizer application techniques due to its lower dry matter content. Separation reduces the size of pumps and tubes required to transport the liquid portion (Monfet et al., 2018). However, most notably, solid-liquid separation allows for crop nitrogen requirements to be met without over application of phosphorus (Vanden Nest et al., 2015). This is due to the unique nutrient profile of the two separated components.

The majority of the phosphorus present in the digestate is located in the suspended solids and is therefore partitioned to the solid component during solid-liquid separation (Lyons et al., 2021). The organic nitrogen content of the digestate – which typically makes up only a small percentage of the digestates total nitrogen content – exists in the suspended solids so it is also separated into the solid component (Czekala, 2022; Lyons et al., 2021). However, with time the suspended solids in the digestate begin to dissolve so to achieve maximum nutrient partitioning, separation should take place as soon as possible (Lyons et al., 2021). The solid component of separated digestate can be used as an organic fertilizer and its benefits are comparable to solid animal manure (Möller & Müller, 2012; Valentinuzzi et al., 2020). Incorporation of solid digestate into soil can improve soil health. Much of the nitrogen present in the digestate is partitioned to the liquid component (Lyons et al., 2021). The liquid component contains little phosphorus which makes it well suited to meet crop nitrogen requirements without increasing the phosphorus load applied (Vanden Nest et al., 2015). The liquid digestate has been found to produce similar crop yields to synthetic fertilizers (Möller & Müller, 2012; Valentinuzzi et al., 2020).

Two common methods used for solid-liquid separation include the screw press separator and decanting centrifuge. In a review paper, Lyons et al. (2021) found that decanting centrifuges are more effective at removing dry matter from digestate while screw press separators are a more affordable option. When combined with coagulant the efficiency of the screw press separator can be greatly increased (Akhlar et al., 2017).

2.3 The DNDC Model Framework

To model the biogeochemical processes which occur in agroecosystems, the DNDC model contains several sub-models which simulate different processes. The soil climate, crop growth,

and decomposition sub models are initially executed by the model framework (He et al., 2019; Institute for the Study of Earth, Oceans and Space, 2012). Using the outputs of the initial sub models the nitrification, denitrification, and fermentation sub-models are initiated. The second set of sub models are initiated simultaneously to estimate the carbon dioxide, methane, ammonia, nitric oxide, nitrous oxide, and dinitrogen emissions occurring within the system. The initial sub models require the major ecological drivers to be defined by the user.

The major ecological drivers such as climate, soil, crop or vegetation, and management practices must be defined by the user to operate the DNDC model (Institute for the Study of Earth, Oceans and Space, 2012). At minimum, daily climate data must include the Julian day, mean temperature, and precipitation of the site. Additional data such as minimum and maximum temperature, radiation, windspeed, and humidity can also be included. A number of sub models within the DNDC framework utilize these parameters such as the crop growth sub model which is simulated at a daily time step (Institute for the Study of Earth, Oceans and Space, 2012). The simulated crop growth has an influence on the carbon and nitrogen cycling in the soil profile as well as the soil water balance. The soil climate and decomposition activity sub models are also simulated based on the ecological drivers. The outputs of the soil climate and decomposition sub models are utilized to determine the soil environmental factors which are utilized by the secondary set of sub models.

The soil environmental factors include temperature, moisture, pH, redox potential (Eh), and substrate concentration and are used to determine the rate at which soil biogeochemical processes occur (Institute for the Study of Earth, Oceans and Space, 2017)). Some of the soil environmental factors are defined by user input. The DNDC model requires the user to define, at a minimum, the soil texture, saturated hydraulic conductivity, field capacity, porosity wilting point, clay fraction, bulk density, organic carbon, and pH of the soil. The remaining soil environmental factors are determined through internal model processes. Soil temperature is determined by the model through heat transfer calculations which utilize user defined soil property data. The calculated soil temperature is a function of soil depth. In the DNDC model, the rate at which reduction-oxidation reactions, such as denitrification, occur is governed by the Eh of the soil. This is determined based on the Nernst equation (Grant et al., 2016). Soil pH is tracked in DNDC through daily accounting of hydrogen ions (Institute for the Study of Earth, Oceans and Space,

2017). The biogeochemical reactions simulated by the model are also influenced by the concentration of substrates present in the soil. Substrate concentrations are modeled in DNDC through the accounting of dissolved organic carbon, ammonium, and nitrate concentrations at a daily timestep. Soil moisture calculations are determined based on the water movement through the soil profile.

2.3.1 *Water Movement in the DNDC Model*

With all process-based models there exists a tradeoff between accuracy and computational capacity; DNDC is no exception to this. In the DNDC model, water flow through the soil profile is determined via a cascade flow algorithm (Smith et al., 2020). This assumes, on an hourly basis, that when a soil layer is above field capacity it will drain to the layer below it (Grant et al., 2016; Smith et al., 2020). Each layer in the soil profile will drain until it returns to field capacity. In the cascade flow algorithm, the rate at which the water moves through each soil layer is governed by the soil's hydraulic conductivity (K) as determined by the following equation:

$$K = K_{SAT} \left(\frac{\theta - \theta_r}{\theta_s - \theta_r} \right)^{3.5} \quad (1)$$

where K_{SAT} is the hydraulic conductivity of the soil at saturation, θ represents the soil water content, and θ_r and θ_s represent the residual and saturated soil water content, respectively (Smith et al., 2020).

Water movement through preferential flow has been identified as a weakness in DNDC's soil hydrology framework (Jiang et al., 2023; Uzoma et al., 2015). This is displayed in DNDC's overestimation of soil moisture contents during dry periods – a finding attributed to the inability of DNDC to simulate infiltration in cracked clay (Uzoma et al., 2015). It has been recommended that further research be conducted to explore the simulation of preferential flow within DNDC in order to improve the overall timing of water losses (Smith et al., 2020). The movement of water within the DNDC model is also used to determine the movement of nitrogen in the soil profile.

2.3.2 *Nitrogen Losses in the DNDC Model*

The DNDCv.CAN model estimates nitrogen losses from multiple pathways. The model simulates gaseous nitrogen losses from ammonia, nitrous oxide, nitric oxide, and nitrogen gas. In 2016, a new ammonia volatilization sub-model was developed to better estimate nitrogen losses during the field application of slurry (Congreves, Grant, et al., 2016). The new sub-model accounts for slurry pH, dry matter content, nitrogen content, and total ammonia nitrogen which improved the model's prediction of cumulative ammonia losses and thereby cumulative nitrogen losses. While the ability of DNDC to simulate cumulative nitrogen losses to runoff has been found to be satisfactory, it currently lacks the ability to accurately model the timing of nitrogen losses to runoff (Smith et al., 2020).

Nitrogen leaching in DNDC is governed by a set of assumptions. Approximately 90% of the nitrate present in soil is assumed to be transferred vertically through the soil profile when in the presence of a positive water flux (Smith et al., 2020). The movement of the nitrate is limited by the adsorptive capacity of the soil (Grant et al., 2016). DNDC assumes 10% of nitrate is transported by preferential flow out of the soil profile and into the groundwater (Grant et al., 2016; Smith et al., 2020). The DNDC model also faces some challenges when modeling nitrogen leaching. A study conducted in 2021 found DNDC was unable to produce accurate results for nitrate leaching in soils with very low nitrogen contents (J. Zhang et al., 2021). The authors hypothesize this is due to an underestimation of the availability of inorganic nitrogen during periods of nitrogen stress.

Chapter 3 – Methodology

The methods and datasets utilized in this study are presented in Chapter 3. The region explored in this research is introduced in section 3.1. The modeling inputs and outputs are outlined in sections 3.2 and 3.3, respectively. The calibration procedure used to develop the models used in this thesis is presented in section 3.4. Section 3.5 presents the scenario modeling framework used. Finally, section 3.6 defines the metrics used to assess the results of this work.

3.1 Study Region

Ontario is home to over a quarter of Canadian farms (Government of Canada & Canada, 2022). The most abundant crop types in Ontario, by seeded area, include corn and soybeans. In 2021, approximately 5 million acres – over half of the province's total cropland – were dedicated to the production of corn and soybeans. The Ontario Ecological Land Classification System separates the land in Ontario into three distinct ecozones: The Hudson Bay Lowlands, the Ontario Shield, and the Mixed wood Plains (Government of Ontario, 2024). The climate throughout the ecozones in Ontario varies greatly with annual average temperature ranging from -5.1 to -2.2°C in the northern regions and 6.3 to 9.4°C in the southern regions (Government of Ontario, 2024). Growing season length varies from 65 to 243 days throughout the province. The majority of Ontario's cropland is located in the mixed wood plains ecozone – which encompasses the southern portion of the province – due to its preferable growing conditions. In addition, soil types vary greatly throughout the province (Soil Landscapes of Canada Working Group, 2010).

Given the variability in climate, soil, and land use, there is heterogeneity in the nitrogen leaching potential of the cropland throughout the province. To capture this heterogeneity with the DNDC model, the study area was discretized into smaller units using the Soil Landscapes of Canada (SLC) database (Soil Landscapes of Canada Working Group, 2010). The SLC database is published by Agriculture and Agri-Food Canada (Soil Landscapes of Canada Working Group, 2010). It divides the agricultural areas of Canada into homogenous polygons based on common soil and landscape attributes as identified by historic soil survey maps (Agriculture Agri-Food Canada, 2021). Soils in the SLC database are discussed further in section 3.2.2. In this work, SLC polygons are referred to interchangeably as regions and sites. A number of studies have utilized the SLC database to discretize the Canadian landscapes for agroecosystem modeling (Banger et al., 2020; B. A. De Laporte et al., 2021; Z. Wang et al., 2021). Conducting this work at

the SLC scale also aligned it with previous research conducted by project collaborators at Agriculture Agri-Food Canada (AAFC) who provided the SLC scale climate and crop yield data used in this thesis.

3.1.1 Spatial and Temporal Modeling Domain

To ensure only highly agricultural SLC polygons were included in this work, a minimum crop growth threshold for each SLC polygon in Ontario was employed. To be included, a polygon had to contain at least 100 hectares of corn cropland and 100 hectares of soybean cropland during the 2021 growing season, as modeled after a 2020 study which also modeled corn and soybean crops in Ontario at the SLC scale (Banger et al., 2020). The area of corn and soybean cropland in each SLC polygon were determined using the 2021 Annual Crop Inventory (ACI) dataset – an annual land cover dataset (Agriculture and Agri-Food Canada Science and Technology Branch, 2021). The ACI dataset divides the Canadian landscape into 73 land classification types at a 30m spatial resolution. There are 55 crop types identified by unique ACI codes in the dataset including corn (ACI code = 147) and soybean (ACI code = 158). There were 263 polygons which satisfied the minimum crop growth threshold, and the soil constraints discussed in section 3.2.2. The corn and soybean cropland across the study region is shown in Figure 3a, and the 263 SLC polygons used in this research are shown in Figure 3b.

The DNDC model was run over a 21-year period, spanning from January 1, 2001 - December 31, 2021. The first 10 years of the simulation (2001 - 2010) were used as a spin-up stabilization period to decrease the influence of the initial conditions on model outputs. The simulation period immediately followed the spin-up stabilization period and spanned from January 1, 2011, to December 31, 2021. Only the results of the simulation period are presented in this work.

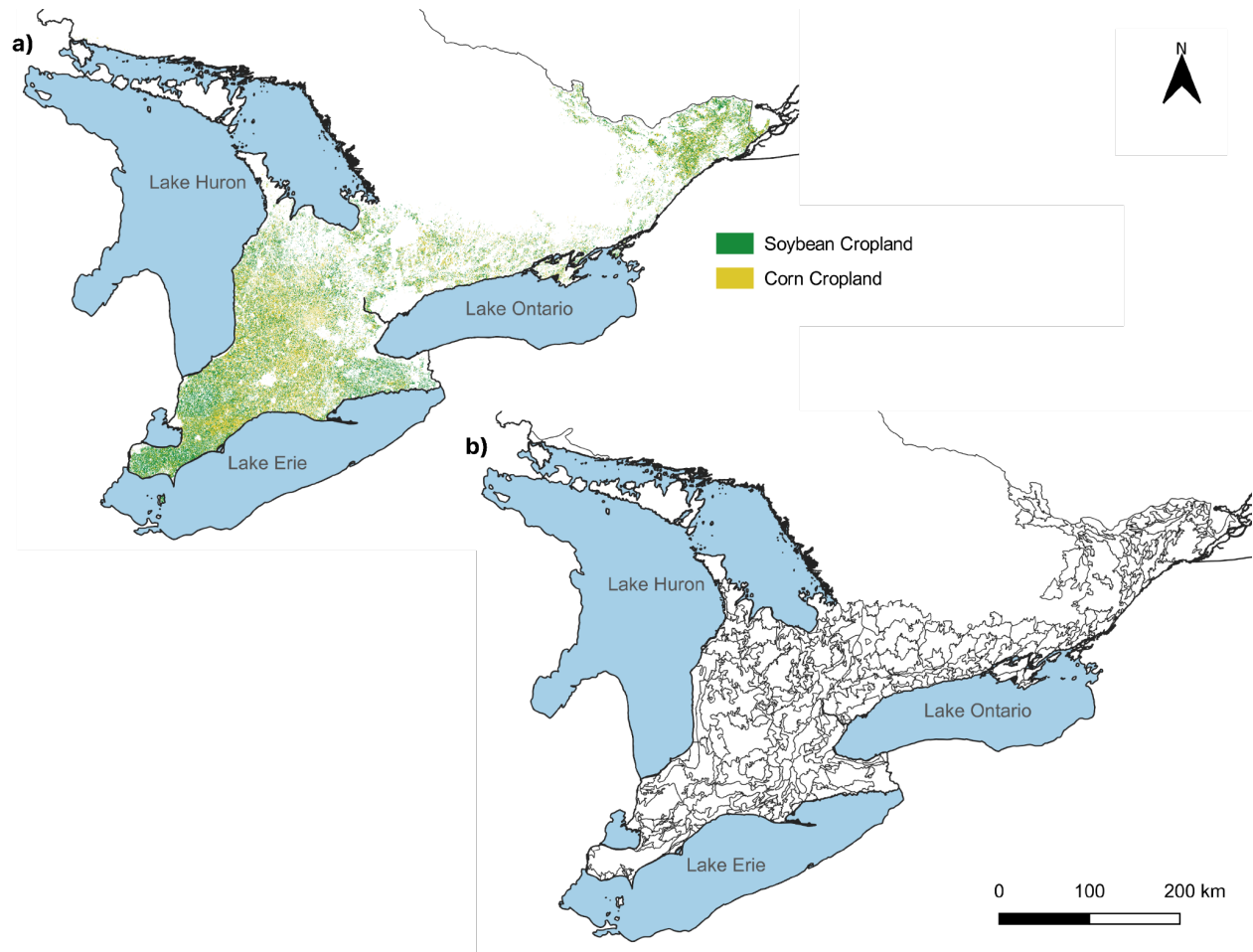


Figure 3: Study region. (a) The corn and soybean cropland within the study region as based on data from the 2021 Annual Crop Inventory dataset (Corn code = 147, soybean code = 158) (Agriculture and Agri-Food Canada Science and Technology Branch, 2021). (b) Discretization from the Soil Landscapes of Canada 3.2 database (Soil Landscapes of Canada Working Group, 2010).

3.2 Input Data for the DNDC Model

3.2.1 Climate Inputs

The climate data used in this project was provided by Agriculture and Agri-Foods Canada. The dataset includes daily climate from January 1, 2001, to December 31, 2021, aggregated to the SLC polygon scale. The dataset contains daily maximum temperature, minimum temperature, radiation, humidity, precipitation, and wind speed.

3.2.2 Soil Inputs

The soil data used in this project was gathered from the SLC database (Soil Landscapes of Canada Working Group, 2010). The SLC database was built upon existing soil surveys which documented the properties of soils across Canada and classified them by soil codes. The SLC database identified which soil codes are present within each polygon. The coverage of each soil type within the polygon (by % area of polygon covered) is included, however, it is not spatially explicit. The database's soil layer table specifies the properties of each soil type. There are multiple soil horizons identified for each soil type, however in this thesis only horizon A – the uppermost soil layer – was considered for each soil type.

To fulfill the input requirements of the DNDC model I collected the field capacity, wilting point, porosity, clay content, bulk density, organic carbon content, and pH for each soil in the study region. Over 1300 distinct soil types were identified in the 263 polygons explored in this work. In addition to the soil properties, the DNDC model also requires the texture code for each soil to be specified. Each soil was connected to its corresponding USDA texture code by project collaborators at AAFC. Once all of the soils present within the study region were identified, I then altered the SLC data, as outlined below, to meet the input requirements of the DNDC model and to remove any inaccurate values from the data.

The values for field capacity and wilting point were converted from volumetric units to water filled pore space using the following equation (Fichtner et al., 2019; Robertson & Groffman, 2024):

$$\text{Water Filled Pore Space} = \frac{\text{Volumetric Water Content}}{1 - \frac{\text{Bulk Density}}{\text{Particle Density}}} \quad (2)$$

where water filled pore space and volumetric water content are both fractions, bulk density is in units of grams per cubic meter [g/cm^3], and particle density is $2.65 g/cm^3$. Soil porosity was calculated using the following equation:

$$\text{Porosity} = 1 - \frac{\text{Bulk Density}}{\text{Particle Density}} \quad (3)$$

where bulk density is in units of g/cm^3 , particle density is $2.65 g/cm^3$, and porosity is a fraction. The clay and organic carbon content of each soil was changed from percent units to fractions (values between 0 and 1) to match the input requirements of DNDC.

The saturated hydraulic conductivity (K_{sat}) values reported in the SLC dataset were replaced using pedotransfer functions to improve the reliability of the values. The process of replacing the K_{sat} data is discussed further in section 3.3.2.1. Soils with wilting points and field capacities less than zero were removed from the dataset as these values were deemed unrealistic. Soils with bulk densities below $0.5g/cm^3$ were also removed from the dataset as they likely correspond to peatlands which are not of particular interest in this work. The DNDC model is unable to simulate soils with organic carbon (SOC) fractions equal to 0. Therefore, all SOC fractions reported as 0 were replaced with 0.003 because this was the lowest non-zero SOC value reported by the dataset. The SLC database also contains a number of soils with large SOC fractions, however, SOC contents above 0.04 are atypical for cropland (Edwards, 2022). To reflect this, all soils with SOC fractions above 0.04 were removed.

The DNDC model provides users with the ability to simulate a homogenous soil profile – uniform soil properties through the 2m profile – or a heterogeneous soil profile – a profile with up to 10 layers of user defined thickness that each contain different properties. The thickness of the user defined layers in the heterogeneous soil profile must equal 2m. There are two processes that occur during the simulation of a homogeneous soil profile that do not occur during the simulation of a heterogeneous soil profile.

The first process is the alteration of K_{sat} within the model. When simulations are conducted using a homogenous soil profile, the inputted K_{sat} value is overwritten by internal pedotransfer functions based on soil texture. The second process that only occurs when simulating a homogeneous soil profile is the stratification of soil organic carbon (SOC) throughout the soil profile. Under a homogenous soil profile, the DNDC model requires the user to input the SOC content of the topsoil layer. The model then applies an internal decay function to reduce the inputted SOC content exponentially throughout the descending soil layers. In this work K_{sat} is a calibrated parameter (calibration is discussed further in section 3.4) and thus must not be overwritten by internal processes. To prevent it from being overwritten, each site was modeled under the conditions of a

heterogeneous soil profile. The heterogeneous soil profile used included 5 uniform layers each 0.2m thick. Each layer in the soil profile contained the same soil properties, except for SOC. The SOC content reported by the SLC database was used as the value for the uppermost soil layer. To mimic the SOC stratification done under homogeneous model conditions, the internal decay function was manually applied to reduce the top layer SOC content throughout each subsequent layer.

3.2.2.1 Saturated Hydraulic Conductivity Calculation

While the SLC database provides soil data coverage across the agricultural regions of Ontario, the accuracy of the reported soil properties can be disputed. Within the dataset, many of the reported soil properties are not the result of direct measurements, but rather, are estimates and given by experienced pedologists at the time of data collection or extrapolation of sampled data points (Soil Landscapes of Canada Working Group, 2010). For the soil properties that are difficult to measure in the field, such as K_{sat} , it is necessary to implement alternative methods of assessment.

Pedotransfer functions enable soil properties to be estimated based on correlations to other properties. In this thesis, the Saxton Rawls pedotransfer functions were utilized to determine the saturated hydraulic conductivity of each soil (Saxton & Rawls, 2006). The Saxton Rawls functions predict the hydraulic properties of a soil using – the more easily obtainable and directly measured – soil texture and organic matter content. While each soil's sand, clay, and silt content are defined in the SLC database, the soil organic matter content is not. Instead, the average organic matter content for each USDA soil texture was used. The Saxton Rawls equations define saturated hydraulic conductivity with the following equation:

$$K_{sat} = 1930(\theta_s - \theta_{33})^{(3-\lambda)} \quad (4)$$

where K_{sat} is saturated hydraulic conductivity [$m\ h^{-1}$], θ_s is the moisture content at saturation (%v), θ_{33} is the field capacity or moisture content at 33 kPa (%v), and λ is the slope of the logarithmic tension-moisture curve. Determination of a soil's saturated hydraulic conductivity using the Saxton Rawls equations required the assessment of a number of intermediate variables which are defined in Appendix A.

3.2.3 Fertilizer Inputs

Crop nutrient requirements are often supplemented through the application of synthetic fertilizer. However, the rate at which synthetic fertilizer is applied varies at the field scale and by crop type. Thus, estimation techniques must be employed to determine the average amount of nitrogen applied to cropland from synthetic fertilizer sources in Ontario. Unlike corn crops which require large amounts of nitrogen fertilizer, soybean crops in Ontario typically do not and so this work assumed no fertilizer application on soybean crops (Bagg et al., 2022). Two methods were used to estimate the average rate of nitrogen fertilizer application to corn cropland in Ontario. The first method utilized government nitrogen application recommendations.

The Ontario Agronomy Guide for Field Crops contains detailed crop management recommendations for all major field crops grown in the province – including guidelines for applying synthetic fertilizer to cropland (Bagg et al., 2022). The guidelines recommend nitrogen application rates to corn cropland based on the nitrogen content of the soil and the predicted corn yield. Soil nitrogen contents can be determined through soil testing and the agronomy guideline recommends using a pre sidedress nitrogen test (PSNT). Province wide PSNT testing is done by OMAFRA (*Nitrogen Status in 2021 Corn Fields*, n.d.). In 2021, the average PSNT value was 13 ppm – slightly higher than the long-term average value of 12 ppm. To estimate the average application of fertilizer to corn crops in Ontario I used an average PSNT value of 12.5ppm. I then calculated the average reported corn yield in Ontario over the 11-year simulation period using crop yield data produced by AAFC, discussed in section 3.3.1. Based on the average PSNT value and crop yield, the recommended rate of nitrogen fertilizer application was approximately $160 \frac{kg\ N}{ha}$. As recommendations often do not reflect practice, a second method which utilized fertilizer sales data was used to estimate fertilizer application to corn crops in Ontario.

In the 2020 - 2021 growing season, the province of Ontario's agricultural market received 270,000 tonnes of nitrogen fertilizer (Statistics Canada, 2024b). Using the assumption that all nitrogen fertilizer shipped to Ontario in the 2020 - 2021 growing season was utilized within the year of purchase, the quantity of nitrogen applied to corn crops throughout Ontario was estimated. To do this, an average application rate for each field crop in Ontario, aside from corn, was estimated based on Ontario agronomy guidelines (Bagg et al., 2022). This method was used because the recommended nitrogen application rate for corn crops contained the largest variation of all the

field crops examined, therefore taking the average value of the recommended range, as done for the other crops, would likely not reflect actual nitrogen fertilizer allocation to corn in Ontario. Next, the seeded area for each major field crop was from the 2021 Ontario Field Crop Production dataset developed by OMAFRA (OMAFRA, 2024b). The purchased synthetic fertilizer was then distributed to each field crop type, aside from corn, using the estimated fertilizer application rate and total seeded area. The leftover synthetic nitrogen was then allocated to the corn areas of the province, from which the nitrogen application rate applied to corn crops was estimated to be approximately $180 \frac{kg\ N}{ha}$. Details on the seeded crop areas and fertilizer allotment by crop type are provided in Appendix B. The two nitrogen application rate estimates are discussed further in section 3.4.

3.2.4 *Manure Inputs*

In addition to synthetic fertilizer, cropland in Ontario receives supplemental nitrogen from livestock manure application. Estimates of total manure production in Ontario were developed using spatially explicit livestock population data. To do this, I used livestock population data from the 2021 Census of Agriculture (Statistics Canada, 2022b, 2022a, 2022c) that was previously aggregated to the consolidated census subdivision scale and simplified to five broad livestock categories (beef cattle, dairy cattle, hogs, chickens, and broilers) by Malik (2024). I then downscaled the livestock population dataset from the original consolidated census subdivision scale to the SLC scale. The downscaling processes assumed that the livestock within each consolidated census subdivision were evenly distributed throughout the land area. Next, the amount of manure nitrogen present in each polygon was estimated by multiplying the livestock populations by the corresponding nitrogen excretion factors from the TREND-Nitrogen dataset (D. K. Byrnes et al., 2020; D. Byrnes et al., 2022) listed in Table 3. The manure production assessed using 2021 animal population data was assumed to be constant throughout the modeling period (spin-up stabilization and simulation period). The distribution of livestock populations and manure nitrogen is shown in Figure 4.

Table 3: Livestock nitrogen excretion rates. Data from D. K. Byrnes et al. (2020; 2022).

Livestock Type	Nitrogen Excretion Rate ($kg\ N\ animal^{-1}year^{-1}$)
Beef Cattle	69.54
Dairy Cattle	151.73
Hogs	13.80
Chickens	0.58
Broilers	0.41

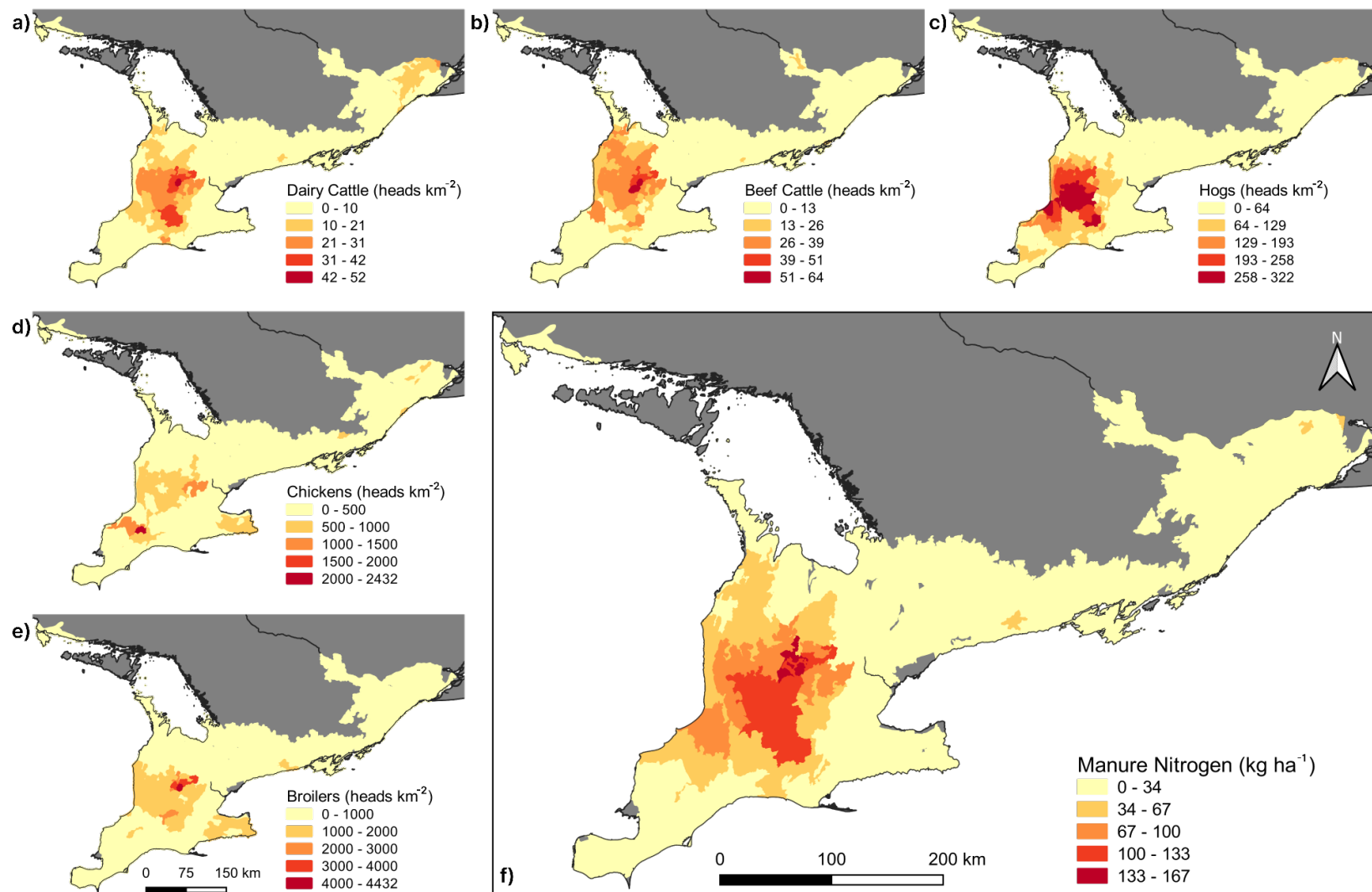


Figure 4: Livestock populations and manure production at the SLC scale. Consolidated census livestock population data downscaled to SLC scale for (a) dairy cattle, (b) beef cattle, (c) hogs, (d) chickens, and (e) broilers. (f) The total nitrogen content of the manure produced is shown as a function of total land area in each SLC polygon.

To simulate the application of manure to cropland, the DNDC model requires the carbon nitrogen ratio (C:N), organic carbon content, organic nitrogen content ($N_{organic}$), inorganic nitrogen content (NH_4), nitrate content (NO_3), percent dry matter (DM), and pH of the manure to be specified. The organic carbon content and $N_{organic}$ were not reported in the databank and were determined by additional calculations which utilized the reported total nitrogen content. Values for C:N, NH_4 , DM, pH, and total nitrogen content were gathered directly from the Government of Ontario's AgriSuite Organic Amendment March 2024 Databank (OMAFRA, 2024a).

The Government of Ontario's AgriSuite Organic Amendment March 2024 Databank includes laboratory analysis results of over 12,000 manure samples of various origins (Brown, 2021). The values reported in the Organic Amendment Databank correspond to the manure samples at the time of application. Thus, nutrient losses, and other property transformations, which occur as a result of manure handling and storage are accounted for in the reported values. The average properties for each manure type are reported in two categories: liquid and solid. To obtain a single set of manure characteristics for each livestock category, the average – weighted by the number of samples – of the reported liquid and solid manure properties was taken. This method assumes the number of samples is reflective of the popularity of solid and liquid manure handling processes for each livestock type. Details on the average reported liquid and solid manure types for each livestock category are outlined in Appendix C. The average manure properties used in this work are outlined in Table 4.

The organic carbon content for each manure type was calculated as the product of the average total nitrogen content and C:N for each livestock type. As the average reported manure NO_3 content in the database was either zero or near zero for all livestock types, it was assumed to be 0 for all manures modeled in this thesis. The $N_{organic}$ of each manure was determined using equation 4.

$$N_{organic} = 1 - NO_3 - NH_4 \quad (5)$$

Table 4: Manure properties by livestock type used as inputs for DNDC model. Broilers and chickens are grouped together in the reporting of manure properties. The dry matter content is defined as the weight of the water in the sample to the weight of the total sample.

Type	NH_4	$N_{organic}$	DM	C:N	pH
Unit	% N_{total}	% N_{total}	%	-	-
Beef	21.35	78.65	26.58	14.59	7.7
Dairy	37.31	62.69	11.53	13.99	7.3
Hogs	64.46	35.54	4.29	2.99	7.6
Chickens	22.42	77.58	56.38	6.82	7.6

To reflect the spatial distribution of livestock types across the province and the variation in the manure properties of different animals, average manure properties were calculated for each site. Average manure properties for each site were determined by taking a weighted average, by SLC polygon livestock populations, of the manure properties outlined in Table 9.

3.2.5 Digestate Inputs

Digestate applications were simulated in the DNDC model using the same process as the manure applications. Thus, digestates simulations required the same properties to be defined as manure simulations and were determined using the method outlined in section 3.3.5. The general set of digestate properties used to model all digestate applications in this work is outlined in Table 5. Additional information about the liquid and solid anaerobic digestate properties used to obtain the average values reported in Table 5 is included in Appendix C.

Table 5: General digestate properties used as inputs for the DNDC model.

Type	NH_4	$N_{organic}$	DM	C:N	pH
Unit	% N_{total}	% N_{total}	% wb	-	-
Anaerobic Digestate	49.24	50.76	10.10	6.13	7.9

3.3 Output Datasets

3.3.1 Reported Crop Yields

The observed crop yield data was compiled, and provided for us in this project, by Agriculture and Agri-Foods Canada. The dataset includes reported annual crop yield data aggregate to the SLC polygon scale. The crop yields provided by Agriculture and Agri-Foods Canada are provided in units of kilogram per hectare of cropland (kg/ha). As the DNDC model reports crop yields in units of kilograms of carbon per hectare, all modeled yields reported in this thesis are converted to kilograms per hectare, using the following conversion recommended by DNDC model developers:

$$\frac{kg}{hectare} = \frac{1}{0.4} * \frac{kg Carbon}{hectare} \quad (6)$$

where the 0.4 is the conversion factor used to find crop yield in kilograms per hectare for a crop with an approximate moisture content of 13% moisture content (*Guidance document for DNDCv.CAN parameters*, 2023).

3.3.2 Observed Nitrogen Leaching Data

Daily nitrogen leaching lysimeter data gathered near Elora, Ontario between November 8, 2018 and April 28, 2022 was provided for use in this thesis by Dr. Claudia Wagner-Riddle (C. Wagner-Riddle, personal communication, February 5, 2024). The daily data was aggregated by year to get annual leaching values. Annual leaching values for years 2018 and 2022 were not used in this thesis as they were not complete years of data. The annual leaching values for years 2019, 2020, and 2021 were used in this thesis to check that the magnitude of nitrogen leaching values reported by the DNDC model for the sites near Elora, Ontario was representative of reality.

3.4 Sensitivity Analysis and Model Calibration

In this work a DNDC model was developed for each of the 263 sites. Calibration techniques were utilized to obtain an optimal set of parameters for each model. The model parameters which remain constant throughout all model runs are outlined in section 3.3.1. The parameters selected to be calibrated are discussed in section 3.3.2. A sensitivity analysis, discussed in sections 3.3.3 and 3.3.4, was then undertaken to explore the influence that various crop, soil, and management parameters had on modeled crop yields in the DNDC model. Finally, the model was calibrated to match observed crop yields, discussed in Section 3.3.5.

3.4.1 *Baseline Modeling Framework*

All model executions were conducted using a corn-soybean-corn-soybean rotation as this was the most commonly employed crop rotation for corn and soybeans grown in Ontario between 2017 and 2019 (Agriculture and Agri-food Canada, 2023). Additionally, all model executions adhered to conventional management practices. In Ontario, conventional tillage for corn crops typically involves moldboard plowing in the fall and a secondary tillage event in the spring (Bagg et al., 2022). To simulate this in DNDC, a disk/chisel tillage event was scheduled before seeding on April 14th at a depth of 15cm, and a moldboard tillage event was scheduled post-harvest on October 15th at a depth of 20cm. Soybeans in Ontario are typically grown with no-till systems and to model this no additional tillage was added before planting or after harvesting soybean crops.

Modeled cropland received a single application of synthetic nitrogen fertilizer in corn years on April 14th, before the land was seeded. Urea fertilizer was used for all synthetic fertilizer applications as it was the most common fertilizer applied to field crops in Canada in 2021 that was not a custom blend (Statistics Canada, 2022d). Urea fertilizer was applied using injection, which when used in conjunction with the scheduled tillage event on April 14th can be considered as incorporation application. Manure or digestate applications were not included in the sensitivity analysis or calibration model runs.

3.4.2 *Parameter and Parameter Range Selection*

A subset of model parameters associated with modeled crop yields were selected for the sensitivity analysis. Parameters in the selected subset fall into four broad categories: soil parameters, corn parameters, soybean parameters, and crop management parameters. A range of possible values was required for each parameter within the selected subset. A number of methods were used to develop ranges for the 20 parameters in the selected subset.

The soil properties explored in the sensitive analysis include saturated hydraulic conductivity, field capacity, clay fraction, bulk density, organic carbon, pH and *Delta*. The soil parameter ranges were determined using the soil dataset. The soil dataset links multiple soil types to each site. Additionally, each site contains a varying number of soil types. To capture the heterogeneity of the soils, present at each site, as well as the heterogeneity of each site across Ontario, a unique soil parameter range was developed for each site in Ontario. For each soil property, the maximum

and minimum value across all soil types observed at each site were used as the range. For sites with only one soil type, a 10% buffer was used to expand each soil parameter range. Porosity was excluded from the tested parameters as it is based on the soils' bulk density. Wilting point was also excluded from the tested parameters and instead replaced with an intermediate value referred to as *Delta*, defined in equation 11.

A soil will always have a wilting point less than its field capacity. As each site has multiple soil types and the field capacity is selected from the range of possible field capacity values at each site, if the same method were used to determine wilting point there is potential for a wilting point to be selected that is larger than the selected field capacity. To avoid this an intermediate variable called *Delta* was created for each soil in the soil dataset and used as a variable in the sensitivity analysis in place of wilting point. In this thesis *Delta* is defined as,

$$Delta = \frac{wilting\ point}{field\ capacity} \quad (7)$$

and was calculated for each soil at each site. The range of *Delta* was defined as the minimum and maximum *Delta* observed at each site. The wilting point was then calculated after the parameter selection process, based on the selected field capacity and *Delta* values.

Table 6: Soil parameters explored in sensitivity analysis.

Parameter	Minimum	Maximum	Reference
Bulk density	Site dependent		(Soil Landscapes of Canada Working Group, 2010)
pH	Site dependent		(Soil Landscapes of Canada Working Group, 2010)
Clay fraction	Site dependant		(Soil Landscapes of Canada Working Group, 2010)
Field capacity	Site dependent		(Soil Landscapes of Canada Working Group, 2010)
Delta	Site dependent		(Soil Landscapes of Canada Working Group, 2010)
K_{sat}	Site dependent		(Soil Landscapes of Canada Working Group, 2010)
Top layer SOC	Site dependent		(Soil Landscapes of Canada Working Group, 2010)

The corn parameters selected for the sensitivity analysis include the maximum grain yield, accumulative temperature, water requirement, and root depth. The maximum grain yield parameter determines the maximum amount of grain biomass that can accumulate throughout a

growing season with ideal conditions. To ensure corn production was not limited by this parameter, it was set based on maximum observed crop yields in Ontario. Many parameter ranges utilized in this work were based on recommended parameters and recommended parameter ranges from model developers as specified in the 'Guidance Document for DNDCv.CAN parameters' model documentation (*Guidance document for DNDCv.CAN parameters*, 2023). The range used for the accumulative temperature parameter was the range recommended in the documentation. The water requirement parameter range was determined by expanding the recommended parameter value by 20%. Finally, maximum root depth was determined based on findings from Fan et al. (2016).

Table 7: Corn parameters explored in sensitivity analysis.

Parameter	Minimum	Maximum	Reference
Maximum Grain Yield	4000	6500	Based on reported crop yields in Ontario.
Accumulative temperature	2150	2700	(<i>Guidance document for DNDCv.CAN parameters</i> , 2023)
Water requirement	120	180	+/- 20% of recommended value (<i>Guidance document for DNDCv.CAN parameters</i> , 2023)
Root Depth	0.7	1.18	(Fan et al., 2016)

The soybean parameters selected for the sensitivity analysis include the maximum grain yield, accumulative temperature, water requirement, and root depth. The maximum grain yield parameter range was selected based on observed crop yields throughout the calibration period. The accumulative temperature range was determined by expanding a model developer recommended value by +/-10% (*Guidance document for DNDCv.CAN parameters*, 2023). The range for the water requirement parameter was the recommended range. Finally, maximum root depth was expanded +/-10% from the recommended value.

Table 8: Soybean parameters explored in sensitivity analysis.

Parameter	Minimum	Maximum	Reference
Maximum Grain Yield	1260	1540	Based on reported crop yields in Ontario.
Accumulative temperature	1395	1705	+/- 10% of recommended value (<i>Guidance document for DNDCv.CAN parameters, 2023</i>)
Water requirement	350	450	(<i>Guidance document for DNDCv.CAN parameters, 2023</i>)
Root Depth	1.2	1.72	(Fan et al., 2016)

The management parameters explored in the sensitivity analysis include fertilizer application, and plant and harvest dates. The corn and soybean plant and harvest dates were both set as a 1 month window of reasonable plant dates in Southern Ontario based on recommendations in the provincial field crop agronomy guidelines (Bagg et al., 2022). The maximum and minimum estimations developed for synthetic fertilizer application to corn crops in Ontario, outlined in section 3.2.3, were used as the calibration range for urea fertilizer application.

Table 9: Management parameters explored in sensitivity analysis.

Parameter	Minimum	Maximum	Reference
Urea Application	160	180	(Bagg et al., 2022; Statistics Canada, 2024b)
Plant Date - Corn	105	135	(Bagg et al., 2022)
Harvest Date - Corn	258	288	(Bagg et al., 2022)
Plant Date - Soybean	105	135	(Bagg et al., 2022)
Harvest Date - Soybean	258	288	(Bagg et al., 2022)

3.4.3 Sensitivity Analysis Site Selection

A pilot study was conducted early on in this project to gain insight into how the modeled crop yield results compared to the observed crop yields in Ontario using a default parameter set. The pilot study provided insights into the ability of the proposed modeling procedure to capture observed crop yield trends. All study sites were run using the same parameter set, aside from site latitude, climate, and soil properties. The most dominant soil type by area at each site was used. The model displayed varying ability to predict observed crop yields at each site. At some sites the model displayed an excellent ability to generate modeled crop yields that closely followed

observed values (less than 1% error in average crop yields over the 11-year simulation period), while others displayed a poor ability (over 80% error in average crop yields over the 11-year simulation period). The poor results of the pilot study indicated that site specific parameter sets were required for the model to capture the crop yields at each site and thus informed the modeling procedure presented in this thesis. The pilot study results were also used to determine the sites modeled in the sensitivity analysis.

Sites that exhibited varying levels of accuracy in the pilot study were selected for the sensitivity analysis to explore different causes of model inaccuracies. Sites where the model produced higher crop yields than the observed yields were marked as overestimations. Sites where the model produced lower crop yields than the observed yields were marked as underestimations. The ten most overestimated, and 10 most underestimated sites were selected for further consideration. Within each category – overestimations and underestimations – the sites were ranked from largest percent error to smallest percent error, with the largest percent error receiving the rank 1. This process was then repeated for the ten sites that showed the lowest percent error in the pilot study, or “best” performing sites. The sites in this category were ranked from smallest percent error to largest, with the smallest error receiving the rank 1.

All sites were then ranked, within their category, from most corn and soybean growing area to least amount of corn and soybean growing area. This was done to select sites where corn and soybean crops were abundantly grown to ensure the reported crop yields in these regions stem from a large sample size. The two rankings, percent error ranking and crop growing area ranking, were then averaged to give each site an overall ranking. The three sites with the lowest overall ranking in each category were selected. However, to ensure that selected sites within each category (overestimated, underestimated, and best performing) were distributed throughout Ontario's agricultural regions, a site was omitted if it was too close to another selected site within the same category. In this case the site with the next best overall ranking would be selected. In total, 3x3 sites were identified to perform a computationally expensive sensitivity analysis.

3.4.4 Sensitivity Analysis Procedure

The Efficient Elementary Effects (EEE) method is an automated sequential screening method for identification of informative parameters (Cuntz et al., 2015; Mai & Cuntz, 2020). The EEE method

of sensitive analysis builds upon the principles of the Morris method to identify informative parameters. The EEE analysis was used to assess the sensitivities of 20 soil, corn, soybean, and crop management parameters based on the influence they exhibited on DNDCv.CAN modeled crop yields at 9 sites in southern Ontario.

There are four major steps in the EEE Analysis. First, the provided subset of parameters (N ; here: $N=20$) is used to generate M sets of $N+1$ parameter sets. The trajectory value M is user-specified depending on the available computational resources- larger values of M provide more reliable sensitivity estimates at the cost of larger computational expenses. Next, the analysis runs the DNDC model for each parameter set and records the modeled crop yield output generated by each parameter set. Then the elementary effects of the tested parameters are calculated. Finally, a threshold value is determined. All parameters with elementary effects values above the threshold value are deemed to be informative, and all below are deemed to be non-informative. The analysis runs iteratively through the four steps, each time removing the informative parameters from the subset of parameters tested — meaning N decreases in each iteration. The process is repeated until no additional informative parameters are identified for two consecutive iterations. In this work, a trajectory value of $M=5$ was used for the first and last iteration. For all other iterations a trajectory value of $M=1$ was used. These settings are recommended by (Cuntz et al., 2015; Mai & Cuntz, 2020).

3.4.5 Calibration Procedure

To obtain an optimal set of the 20 parameters for each site, the DNDC model was calibrated separately for the 263 sites explored in this work. Model calibration was conducted using the OSTRICH optimization and calibration tool (Matott, 2017). The OSTRICH tool is model-independent and operates using a user-specified optimization algorithm, thereby enabling it to be customized to suit a range of applications. In this work the Dynamically Dimensioned Search (DDS) optimization algorithm was selected for use (Tolson & Shoemaker, 2007). The default perturbation value of 0.2 was used. In addition to specifying the optimization algorithm, the user must also define the parameters and associated ranges that are to be calibrated. In this work, OSTRICH was given the subset of parameters and associated ranges used for the sensitivity analysis, outlined in section 3.5.2.

The OSTRICH tool generates input values for the identified subset of parameters, within the provided ranges, and executes the DNDC model with the generated input values. The OSTRICH tool then compares the modeled crop yield to the actual – or observed – crop yields and calculates the model error using a user defined metric. The mean absolute percent error (MAPE) was selected as the metric in this thesis because it combines the overestimated yield values and underestimate yield in an additive way, regardless of sign. The MAPE of the corn yield and soybean yields are calculated separately, and then the arithmetic mean is taken of the two values. This was done to ensure the calibration weights both crops as equal importance, rather than ignoring the soybean yields which tend to be much lower than the corn yields. The metric used in this thesis is defined as,

$$MAPE_{Corn} = 100 \frac{1}{n} \sum_{i=1}^n \left| \frac{Observed\ Corn\ Yields_i - Calibrated\ Corn\ Yields_i}{Observed\ Corn\ Yields_i} \right| \quad (8)$$

$$MAPE_{Soybean} = 100 \frac{1}{n} \sum_{i=1}^n \left| \frac{Observed\ Soybean\ Yields_i - Calibrated\ Soybean\ Yields_i}{Observed\ Soybean\ Yields_i} \right| \quad (9)$$

$$MAPE = \frac{MAPE_{Corn} + MAPE_{Soybean}}{2} \quad (10)$$

where n is the number of years in the simulation, i is the year of the simulation, and MAPE (%) is the metric used by OSTRICH to evaluate and adjust the current input values. The OSTRICH tool performed 500 model evaluations for each site to identify the optimal parameter set using DDS.

3.5 Scenario Modeling Framework

To explore the influence different nitrogen distribution configurations had on nitrogen leaching, a scenario modeling approach was taken. Each scenario was developed using a unique distribution of manure or digestate onto the landscape. In this thesis, the land within the study region upon which manure is applied is referred to as spreadable land. The definition of spreadable land in each scenario varies and is determined as a fraction of the total agricultural area present within each SLC polygon. The agricultural areas of Ontario were defined using the 2021 ACI dataset (Agriculture and Agri-Food Canada Science and Technology Branch, 2021). In this work, the agricultural area of each polygon was assumed to be the total land area excluding: barren regions (ACI code = 30), urban regions (ACI code = 34), shrublands (ACI code = 50), grasslands (ACI

code = 110), wildfire areas (ACI code = 60), wetlands (ACI code = 80), peatlands (ACI code = 85), too wet to be seeded regions (ACI code = 130), and forested regions (ACI code = 200, 210, 220, 230). The agricultural areas of Ontario are illustrated in Figure 5.

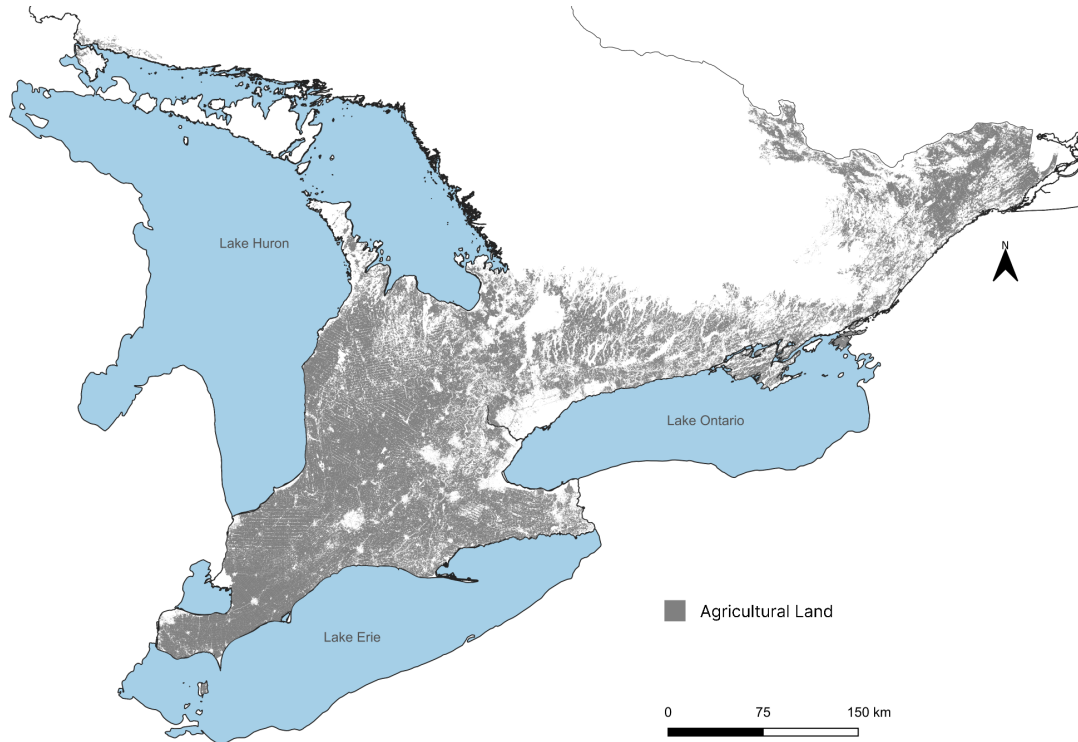


Figure 5: Agricultural areas across study region. Agricultural areas were defined using the 2021 Annual Crop Inventory (Agriculture and Agri-Food Canada Science and Technology Branch, 2021) and criteria outlined in section 3.5.

Five unique nitrogen distribution scenarios explored in this thesis, as outlined in Table 10. Model runs conducted under the conditions of all scenarios utilized the site-specific parameters, as identified by the calibration procedure. The calibration scenario included a single application of synthetic fertilizer to corn crops. Many of the scenarios add additional nitrogen to the crops from manure or digestate sources. In all scenarios, manure and digestate is applied by surface spreading on April 15th in all years.

The first scenario (F) explored the case where there is no manure or digestate application to the landscape. This scenario uses the same conditions as the calibration scenario. The application of manure and digestate is not included in this scenario.

Two manure scenarios (FM) were explored in this work. In both manure scenarios, manure was constrained to be applied within the polygon in which it was produced. This choice was made to reflect the transportation constraints manure is subject to. The first manure scenario (FM1) assumes that the spreadable land in each polygon is equal to 75% of the polygons' agricultural areas. The second manure scenario (FM2) assumes the spreadable land in each polygon is equal to 50% of the polygon's agricultural area. The nitrogen content of the manure produced in, and applied within, each polygon was determined using the method presented in section 3.4.1. The properties of the manure produced in, and applied within, each polygon was determined using the method presented in section 3.4.2. The distribution patterns of manure nitrogen used in scenarios FM1, and FM2 are shown in Figures 6a and 6b, respectively.

Two scenarios were used to explore the impact of digestate use in place of manure. The digestate scenarios simulate corn and soybean cropland throughout a 100km^2 region located in a manure hotspot in Southern Ontario. These scenarios were designed to explore the impact that a theoretical biodigester may have on the landscape. Model runs conducted under the conditions of the biodigester scenarios were done using a subset of SLC polygons. SLC polygons which did not have at least 10% of their area within the 100km biodigester radius were excluded in the digestate scenarios. In this work the digestate properties, defined in Table 5, are assumed to remain constant throughout all sites and scenarios.

The first digestate scenario (FD1) was constructed to explore the nitrogen leaching implications of replacing manure with an equivalent amount of digestate, based on total nitrogen content, without considering the enhanced distribution distance of digestate. In scenario FD1, digestate is constrained to be applied within the same polygon that the manure feedstock was produced in, and the spreadable land is equal to 75% of the agricultural area of each polygon. It was assumed the nitrogen content of the manure is retained in the digestate with no nitrogen losses, and thus FD1 follows the same nitrogen distribution pattern as scenario FM1. The nitrogen distribution pattern of FD1 and FM1 across subsets of sites included in the biodigester scenarios are shown in Figure 6c.

The second digestate scenario represents the case where a large scale biodigester is strategically placed in the center of the manure hotspot. In this scenario it is assumed that all of the manure produced in polygons within a 100km radius of the manure hotspot, is transported to a biodigester. The manure produced within the biodigester radius is transformed to an equivalent amount of digestate, by total nitrogen content, and dispersed evenly to 100% of the agricultural areas within contributing polygons. The digestate is not constrained to be applied within the polygon in which the manure feedstock was produced. It is assumed the nitrogen content of the manure is retained in the digestate with no nitrogen losses. The distribution patterns of digestate nitrogen used in scenarios FD2 is shown in Figure 6d.

Table 10: Nitrogen distribution scenario framework.

Nitrogen Distribution	
F	Synthetic fertilizer application with no manure added to the landscape.
FM1	Manure is distributed evenly within the polygon in which it was produced. Spreadable land is equal to 75% of agricultural areas.
FM2	Manure is distributed evenly within the polygon in which it was produced. Spreadable land is equal to 50% of agricultural areas.
FD1	Digestate is distributed evenly within the polygon in which the manure feedstock was produced. Spreadable land is equal to 75% of agricultural areas.
FD2	Digestate is distributed evenly to all spreadable land within 100km radius of the biodigester.

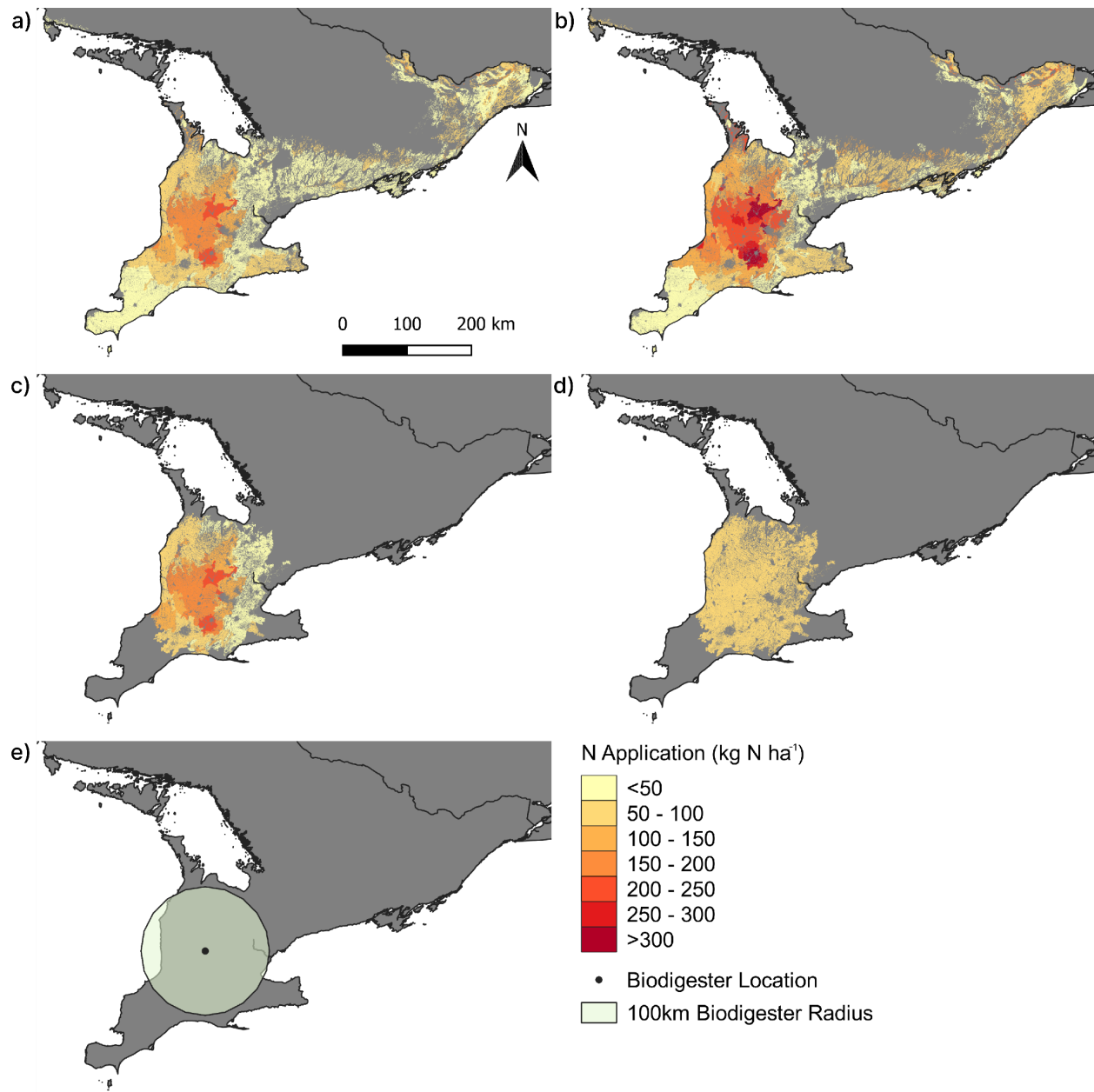


Figure 6: Manure and digestate distribution to agricultural land. Manure scenarios (a) FM1 and (b) FM2 extend across 263 SLC polygons while biodigester scenarios (c) FD1 and (d) FD2 extend across the 95 SLC polygons that are within 100km of the (e) theoretical biodigester location.

In this work, the amount of manure applied to the cropland at each site was a function of the site's agricultural land area and livestock population. It also varied between scenarios based on the assumption of spreadable land. The maximum and minimum rates of total nitrogen application (manure + synthetic fertilizer) are outlined in Table 11.

Table 11: Manure and synthetic fertilizer application range.

	Synthetic Fertilizer + Manure Application ($kg\ N\ ha^{-1}yr^{-1}$)
F	160 - 180
FM1	168 - 411
FM2	170 - 533

A study conducted in 2008 estimated the amount of nitrogen applied to cropland across Canada, at the SLC scale, from synthetic fertilizer and manure sources (Huffman et al., 2008). The study utilized both similar and different methods to the ones used in this thesis and found the combined synthetic fertilizer and manure nitrogen application rate ranged from 25 - 307 $kg\ N\ ha^{-1}yr^{-1}$ for corn crops and between 8 - 314 $kg\ N\ ha^{-1}yr^{-1}$ for all crop types explored. The nitrogen application rates determined in this thesis exceed the rates reported by Huffman et al. The analysis performed by Huffman et al. assumed that the manure present in each SLC polygon was applied to 100% of the cropland in the polygon, while the work in this thesis assumed transportation constraints would limit the amount of cropland manure could be applied to. The analysis by Huffman et al. also accounted for manure losses in pastures and manure storage and handling losses, which the work in this did not.

3.6 Nitrogen Leaching Analysis

The magnitude of nitrogen leaching was assessed for the corn and soybean cropland across the study region under the conditions of all scenarios. The 2021 ACI database was used to determine the amount and distribution of corn and soybean cropland across the region (Agriculture and Agri-Food Canada Science and Technology Branch, 2021). The area of corn and soybean land in each polygon was assumed to remain constant throughout the simulation period.

First, the nitrogen leaching for each hectare of corn and soybean cropland in the study region was assessed. To do this, the average nitrogen leaching rate for each site under the conditions of each section was calculated. It was calculated as the mean value of the nitrogen leaching output of the DNDC model over the 11-year simulation period for each scenario. Next, an average nitrogen leaching value was assigned to each hectare of corn and soybean cropland within the

site. It was assumed that the portion of corn and soybean cropland receiving manure or digestate treatments within each SLC polygon was proportional to the definition of spreadable land in each scenario. For example, scenario FM2 assumed that spreadable land was equal to 50% of the total agricultural areas. Under this scenario, 50% of the corn and soybean cropland in each SLC polygon would receive manure and synthetic fertilizer applications and therefore would be assigned the nitrogen leaching value for scenario FM1. The other 50% of the corn and soybean cropland within the polygon would only receive synthetic fertilizer application and therefore would be assigned average nitrogen leaching value for scenario F. Next, the average nitrogen leaching rate for each SLC polygon was assessed using the mean nitrogen leaching value across the corn and soybean areas in the polygon. The total amount of nitrogen lost annually by leaching from the study region was also estimated. It was determined as:

$$Total\ nitrogen\ lost\ by\ leaching = \frac{1\ kt}{1000000\ kg} \sum_{n=1}^{2,350,935} average\ nitrogen\ leaching * 1ha \quad (11)$$

where, *total nitrogen lost by leaching* is in units of $kt\ Nyr^{-1}$, n is the number of hectares of corn and soybean cropland in the study region, and *average nitrogen leaching* is determined for each hectare of land and varies with scenario in units of $kg\ N\ ha^{-1}yr^{-1}$.

Chapter 4 – Results and Discussion

In Chapter 4 I will outline the results of calibrating the DNDC model and using it to explore the nitrogen leaching losses associated with manure and digestate application. The results of the sensitivity analysis and model calibration are presented in sections 4.1. and 4.2, respectively. The nitrogen leaching losses from the scenario modeling analysis are presented in section 4.3.

4.1 Sensitivity Analysis Results

The EEE sensitivity analysis identified 4 parameters to be informative at all 9 test sites. These include the urea application rate, top layer soil organic carbon (SOC) content, the corn plant date, and corn harvest date. The analysis also revealed 2 parameters which were not informative at any of the test sites. These include the soybean harvest date, and the soil hydraulic conductivity. The results of the sensitivity analysis are displayed in Figure 7. In addition to identifying a number of informative parameters, the sensitivity analysis provided immense insight into the internal processes of the DNDC model not included in published documentation, which aided in shaping many of the methodologies presented in Chapter 3.

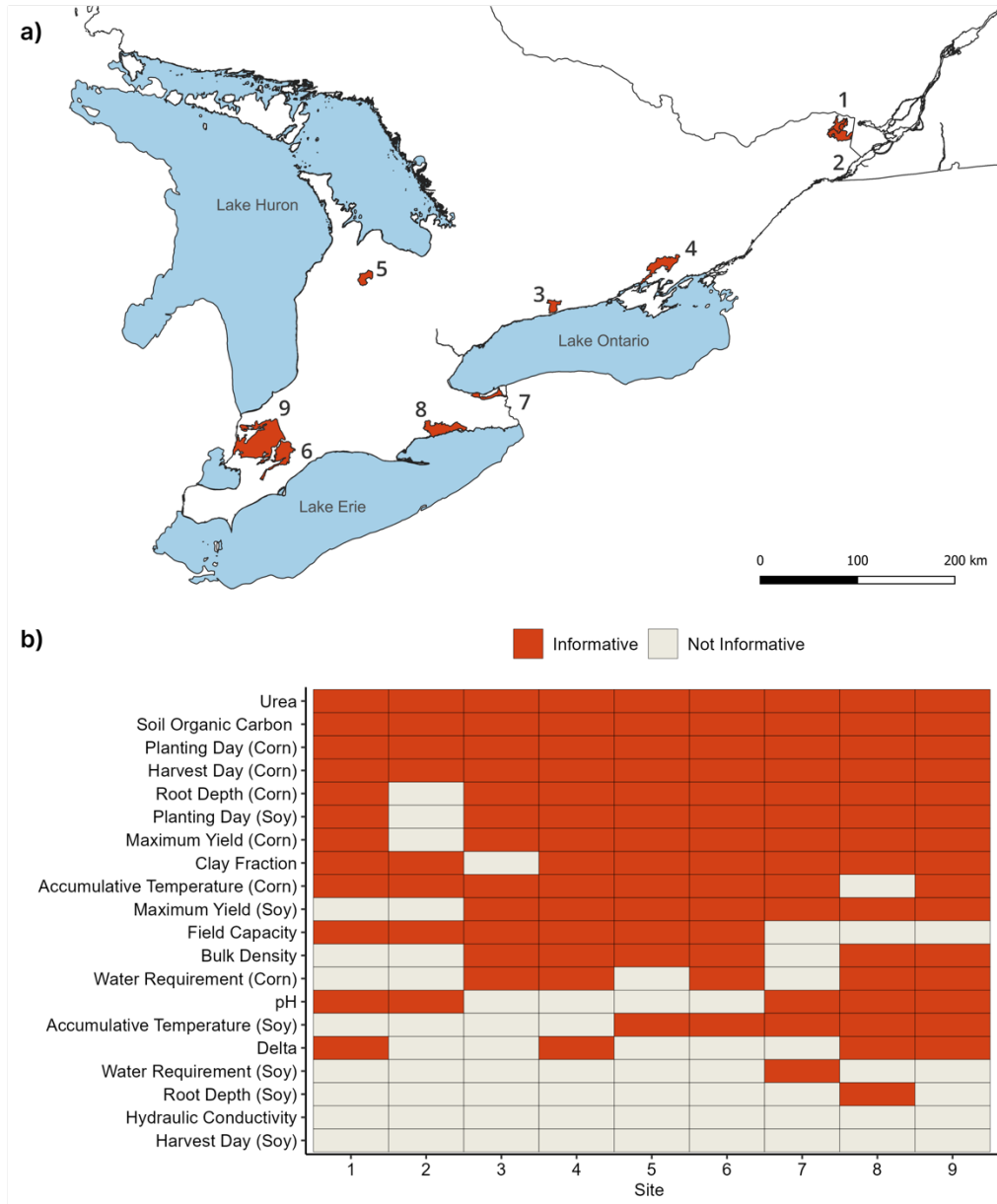


Figure 7: Efficient Elementary Effects sensitivity analysis results. (a) Sites included in the analysis. (b) The informative and uninformative parameters identified at each site.

4.2 Model Performance and Calibrated parameters

Separate models were developed for each site and calibrated independently over an 11-year period spanning January 1, 2011, to December 31, 2021. Using the calibration procedure outlined in Chapter 3, an optimal set of parameters was identified for each site. The optimal parameter

sets were used for all model evaluations conducted in this work. The mean absolute percent error (MAPE), as defined in section 3.4.5, was used to evaluate the performance of the calibration procedure. The calibrated model was able to predict corn, and soybean yields adequately well over the 263 soil polygons and the 11 years of crop yield data, with a median error of 5.8%.

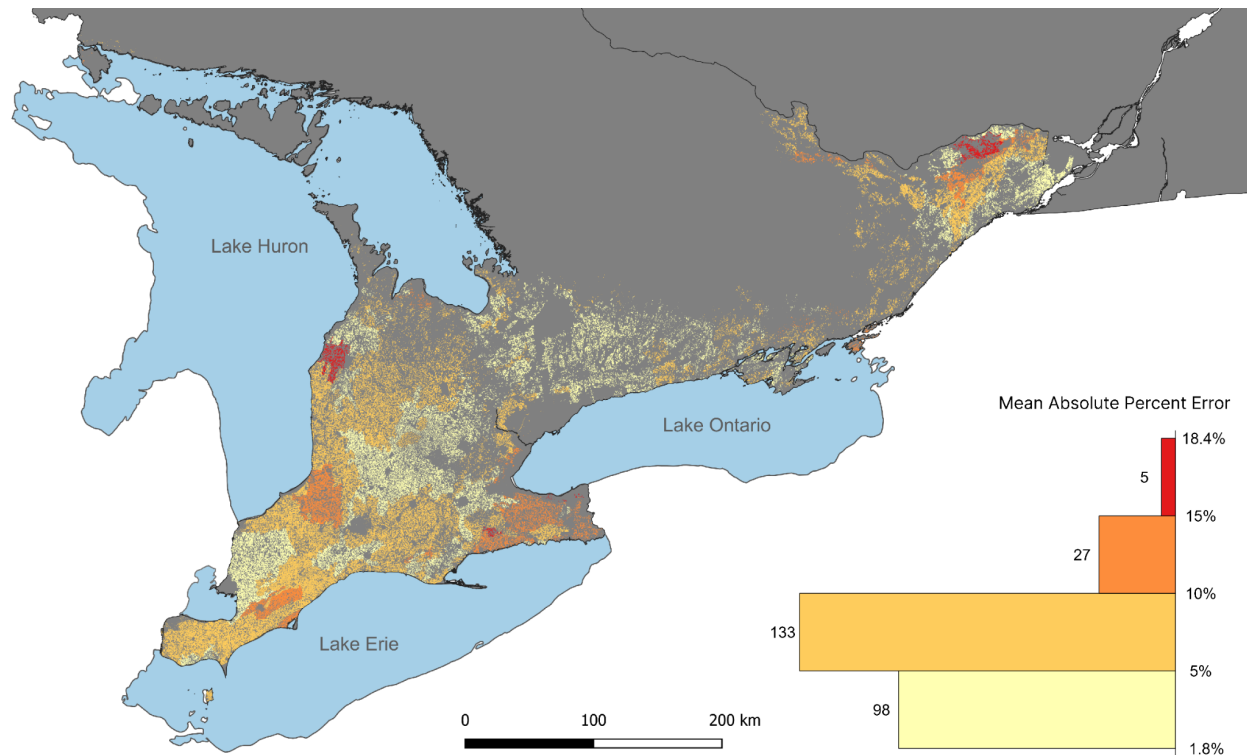


Figure 8: Calibration objective function value across 263 SLC polygons. The mean absolute percent error between calibrated crop yields and observed crop yields was evaluated by the OSTRICH calibration tool.

The median error across all sites was 5.8%. SLC polygon scale data was downscaled to corn and soybean cropland at the 30m scale using the 2021 ACI database (Agriculture and Agri-Food Canada Science and Technology Branch, 2021). Gray areas represent land not included in the modeling domain.

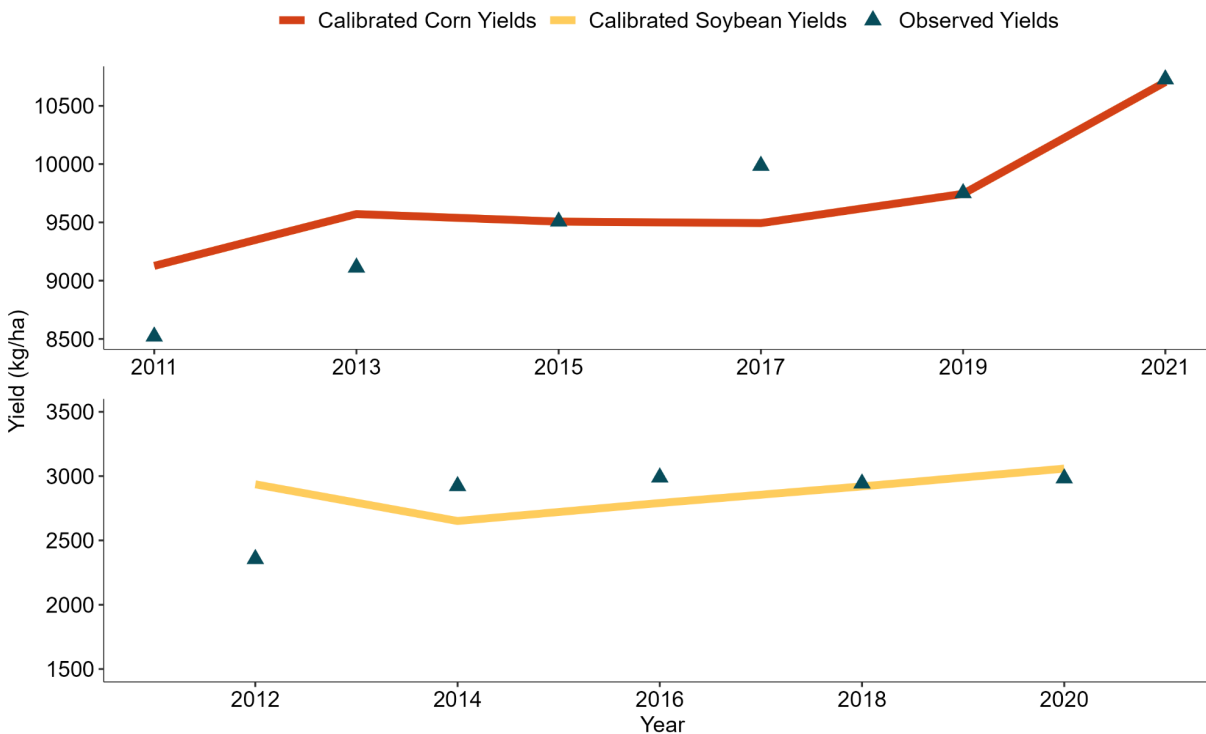


Figure 9: Observed and modeled crop yields over the simulation period. The mean absolute percent error for the site shown in the figure (SLC Polygon ID = 556009) is 5.8% which is equivalent to the median error achieved across all sites.

The calibration procedure identified optimal values for twenty parameters at each site. The calibrated parameters included soil parameters, crop parameters, and field scale management factors and the distribution of optimal values are shown in Figure 10. For all parameters the distribution of optimal values utilized the entire calibration range. However, for the soybean maximum grain parameter, the optimal value selected for most sites was the highest value the calibration range would allow. This indicates that the upper limit of the selected range for this parameter may have limited the performance of the calibration. Additionally, most sites selected the highest value for the soybean plant date parameter which corresponds to May 15th. While extending this range to include later plant dates may improve the calibration performance, it is less common for soybean crops to be planted after May 15th in Ontario as late planting can result in yields reductions (Bagg et al., 2022).

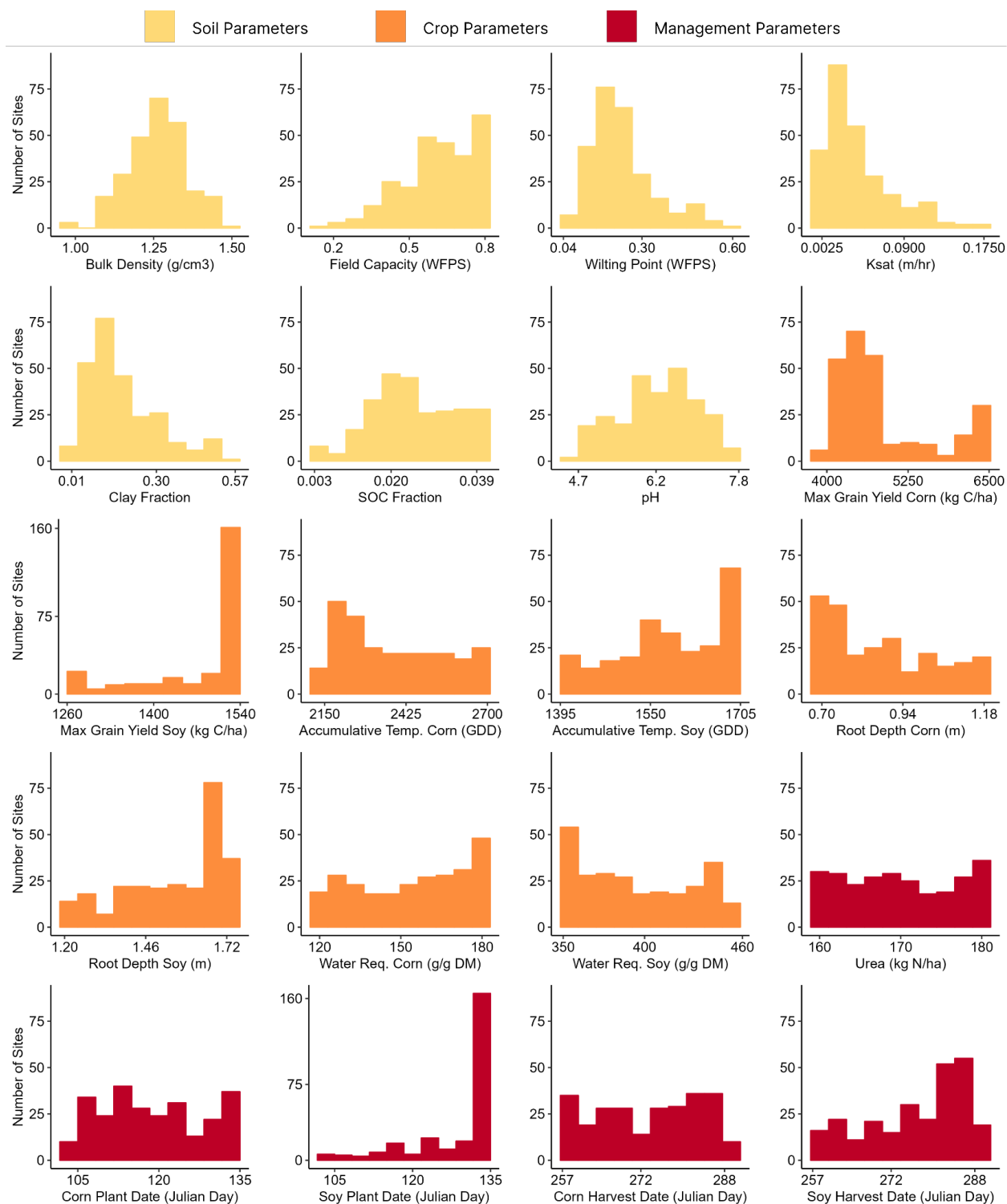


Figure 10: Distribution of optimal parameter values identified through calibration.

The calibrated value for synthetic fertilizer application, or urea application, across the study sites displayed an even distribution throughout the calibration range of all the calibrated parameters, as shown in Figure 10. The calibration range for synthetic fertilizer application was bounded by provincial recommendations ($160 \text{ kg N ha}^{-1}\text{yr}^{-1}$) and an estimate of the purchase synthetic fertilizer allocated to corn crops in Ontario ($180 \text{ kg N ha}^{-1}\text{yr}^{-1}$). The median synthetic fertilizer application rate was $169.5 \text{ kg N ha}^{-1}\text{yr}^{-1}$.

Based on the calibrated application rate and the area of corn cropland in each SLC polygon, $186,840,209 \text{ kgN yr}^{-1}$ of urea fertilizer is needed to meet the corn nitrogen requirements across the entire study region, if no other source of nitrogen is provided. This is equivalent to 69% of the nitrogen fertilizer purchased in Ontario in 2021. As the nitrogen requirements of the corn cropland in the study region is fulfilled by purchased synthetic fertilizer, manure applications to the land are likely done in excess of crop needs.

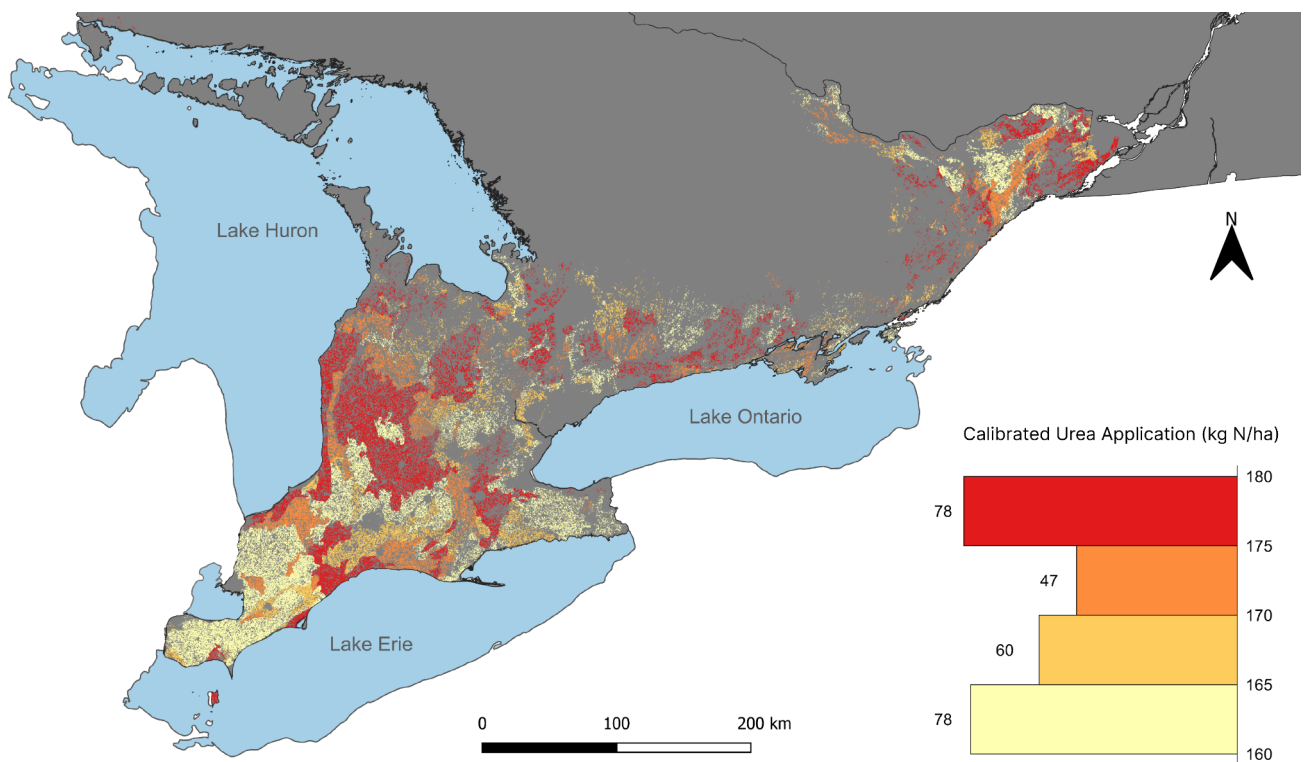


Figure 11: Calibration results for urea fertilizer application in corn years. SLC scale urea calibration results were downscaled to corn and soybean cropland at the 30m scale using the 2021 ACI database (Agriculture and Agri-Food Canada Science and Technology Branch, 2021). Gray areas represent land not included in the modeling domain.

4.3 Nitrogen Leaching Scenario Analysis

The annual nitrogen leaching losses and site average nitrogen leaching rates were assessed for each manure and digestate distribution scenario outlined in section 3.5. The results of the manure distribution scenarios are outlined in section 4.3.1 and were analyzed across all of the corn and soybean cropland in the study region (2,350,935 hectares of land). The digestate scenario results are presented in section 4.3.2 and were analyzed on the corn and soybean cropland across a subset of sites (1,115,617 hectares of land).

4.3.1 Manure Scenarios

I first explored the rate of nitrogen leaching when there is no manure distribution across the landscape and cropland receives only synthetic fertilizer application using scenario F. The amount of fertilizer applied at each site was selected by the calibration which was given a range of $160 \text{ kg N ha}^{-1}\text{yr}^{-1}$ to $180 \text{ kg N ha}^{-1}\text{yr}^{-1}$. The average leaching at each site ranged from $1.38 - 73.03 \text{ kg N ha}^{-1}\text{yr}^{-1}$, with a median value of $26.23 \text{ kg N ha}^{-1}\text{yr}^{-1}$. The highest leaching rates were found in sites located in the Northeast of the study region. The average leaching rate for each site is shown in Figure 12a. The modeled nitrogen leaching rates were of similar magnitude to measured data that was collected under conditions similar to those of scenario F. The measured nitrogen leaching data ranged from 3.9 to $18.2 \text{ kg N ha}^{-1}\text{yr}^{-1}$ (C. Wagner-Riddle, personal communication, February 5, 2024). Two SLC polygons encompassed the region within which the measured data was obtained. The average nitrogen leaching rates produced by the DNDC model for these two SLC polygons was 9.46 and $22.04 \text{ kg N ha}^{-1}\text{yr}^{-1}$. Other DNDC based studies have also simulated the associated nitrogen leaching from corn and soybean crops in Ontario.

A 2020 study explored nitrogen leaching losses throughout a similar study region to the one used in this thesis (Banger et al., 2020). This 30-year modeling study used the DNDC model to simulate corn crops and found average nitrogen leaching rates between $7 - 53 \text{ kg N ha}^{-1}\text{yr}^{-1}$ resulting from synthetic fertilizer applications ranging between $91 - 200 \text{ kg N ha}^{-1}\text{yr}^{-1}$. Similarly, a 2016 DNDC modeling study found nitrogen leaching rates between $19 - 116 \text{ kg N ha}^{-1}\text{yr}^{-1}$ when simulating the application of between $50 - 150 \text{ kg N ha}^{-1}\text{yr}^{-1}$ of fertilizer to a corn and soybean crop rotation (Congreves, Dutta, et al., 2016). While the reported nitrogen leaching losses vary

between studies, it may be attributed to study conditions. Nitrogen leaching losses in agroecosystems can vary based on a number of factors including soil type, climate, crop type, nitrogen application techniques, and nitrogen application rates. Nitrogen leaching losses have been found to increase as a direct result of increased nitrogen application, when applied above the crops nitrogen requirements (Andraski et al., 2000; Congreves, Dutta, et al., 2016; Hoogendoorn et al., 2017; L. Wang et al., 2023).

I then assessed the magnitude of the amount of nitrogen lost across the study region under the conditions of scenario F. The average amount of nitrogen lost by leaching from all the corn and soybean cropland modeled in this thesis (2,356,550 hectares) was $68.57 \text{ kt N yr}^{-1}$. Results of a similar magnitude were reported by a modeling study which utilized the DNDC model coupled with a spatial economic maximization model to estimate nitrogen leaching losses across 270 SLC polygons in southern Ontario (A. De Laporte et al., 2021). The study simulated treatments of synthetic fertilizer comparable to the conditions of scenario F explored in this thesis. The study estimated that across 980,344 hectares (42% of the area covered in this thesis) of corn and soybean cropland, 32 kt N yr^{-1} would be lost annually by leaching. However, the conditions simulated under scenario F are not representative of reality – they lack the addition of manure to the landscape. The application of synthetic fertilizer and manure to the cropland in the study region was explored through scenarios FM1 and FM2.

The magnitude of nitrogen leaching which occurs as a result of synthetic fertilizer and manure application to cropland was assessed under two manure distribution configurations. In both scenarios, manure was constrained to be applied within the polygon in which it was produced to restrict the movement of manure on the landscape. However, as the size of the SLC polygons are larger than the distance over which manure is typically transported, additional transportation constraints were implemented. In scenarios FM1 and FM2 it was assumed that the manure within each polygon could only be applied to a fraction of the polygon's agricultural land area.

When the manure was distributed across 75% of the agricultural areas in each site (FM1), the total amount of nitrogen applied to corn and soybean cropland ranged from $168 \text{ kg N ha}^{-1}\text{yr}^{-1}$ to $411 \text{ kg N ha}^{-1}\text{yr}^{-1}$. The average nitrogen leaching rates across the 263 simulated sites ranged from $3.39 - 93.98 \text{ kg N ha}^{-1}\text{yr}^{-1}$, with a median value of $31.16 \text{ kg N ha}^{-1}\text{yr}^{-1}$, shown in figure

12b. Under these conditions, an average of $93.22 \text{ kt N yr}^{-1}$ was estimated to be lost across the modeling domain. However, when the manure was distributed to only 50% of the agricultural land in each polygon, as specified by scenario FM2, the total nitrogen application to the corn and soybean ranged from $170 \text{ kg N ha}^{-1}\text{yr}^{-1}$ to $533 \text{ kg N ha}^{-1}\text{yr}^{-1}$. Site average leaching – shown in figure 12c – ranged from 3.41 to $94.58 \text{ kg N ha}^{-1}\text{yr}^{-1}$ with a median value of $32.11 \text{ kg N ha}^{-1}\text{yr}^{-1}$. When the manure was distributed in this way, the average nitrogen lost across the corn and soybean cropland in the study region was $94.87 \text{ kt N yr}^{-1}$.

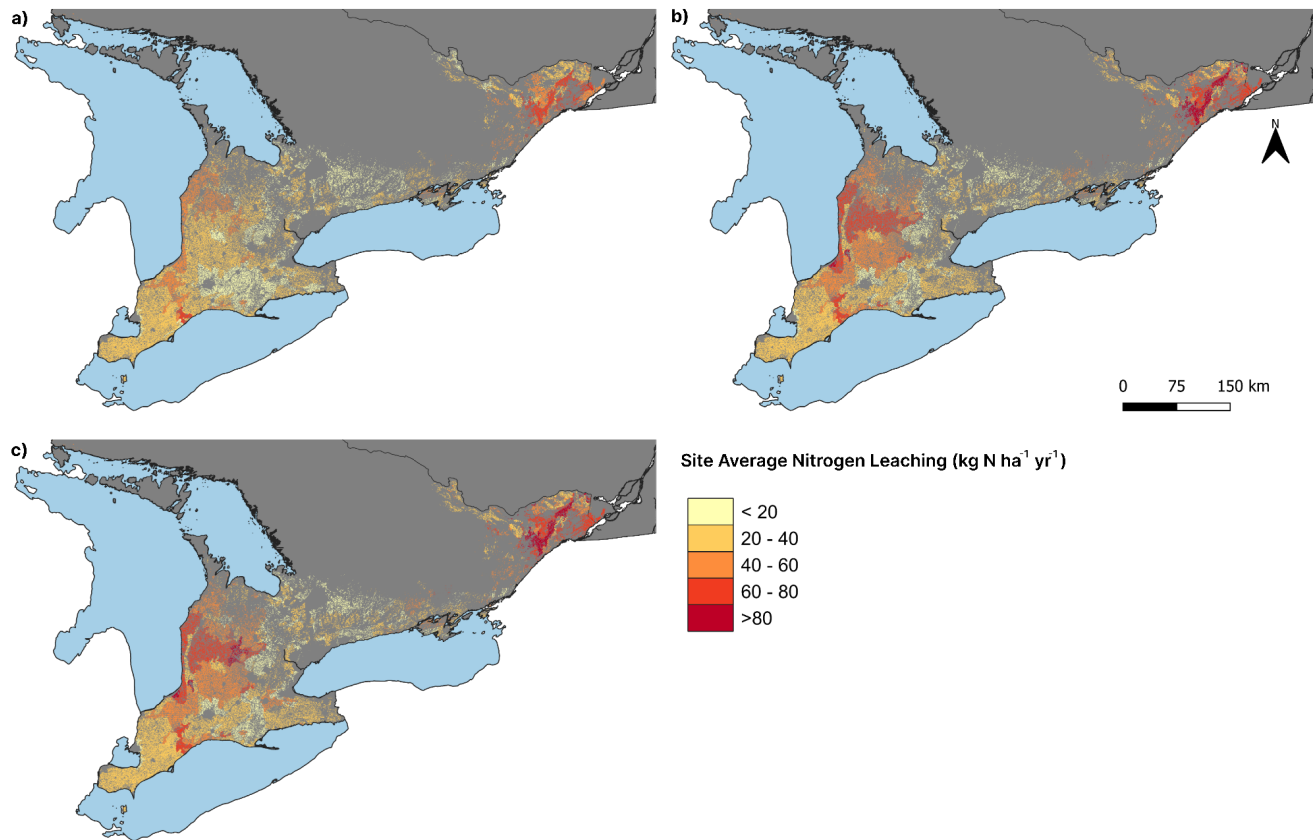


Figure 12: Average nitrogen leaching rate by site for manure scenarios. (a) No manure application, (b) manure spread evenly to 75% of the agricultural land at each site, and (c) manure spread evenly to 50% of the agricultural land at each site.

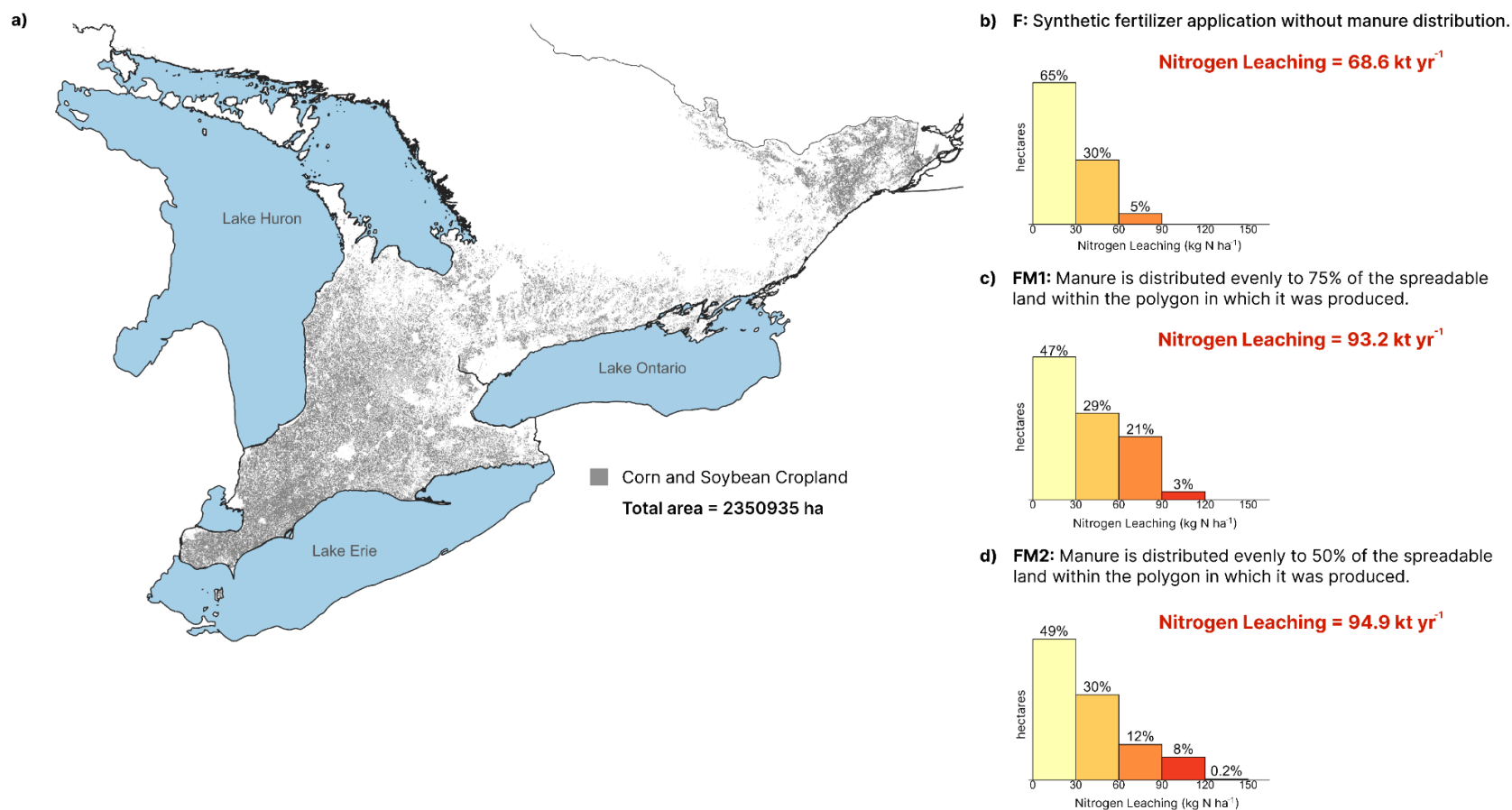


Figure 13: Annual nitrogen leaching losses from manure scenarios. (a) The area included in the manure scenario analysis. The 11-year average annual nitrogen losses from leaching and the leaching rate distribution per hectare of simulated land with (a) no manure application, (b) manure application under the conditions of FM1, and (c) manure application under the conditions of FM2.

The results obtained from scenarios FM1 and FM2 show that as the spreadable land area decreases and thereby the rate of manure application increases, the quantity of nitrogen lost through leaching increases. From this it can be inferred that a wider distribution of manure throughout the landscape can aid in reducing the nitrogen leaching losses. However, economic and logistic factors often limit the feasibility of wider manure distribution.

4.3.2 *Biodigester Scenarios*

I then explored the influence a central biodigester may have when introduced to a manure hotspot in Southern Ontario. A biodigester was assumed to have a feedstock contribution region of 100 km^2 which included 95 SLC polygons. First the case where the manure in each polygon was replaced with an equivalent amount of digestate, by total nitrogen content, and distributed to 75% of the agricultural lands, was investigated using scenario FD1. The application and distribution pattern of nitrogen for scenario FD1 was the same as scenario FM1 (included in this section for comparison), the total amount of nitrogen applied in these scenarios ranged between 9.12 and 244.71 $kg N ha^{-1} yr^{-1}$ over the subset of sites located within the biodigester radius. When manure was applied according to the distribution pattern of FM1, site average nitrogen leaching varied from 3.39 to 88.20 $kg N ha^{-1} yr^{-1}$ with a median value of 30.07 $kg N ha^{-1} yr^{-1}$. However, when the manure was replaced with an equivalent amount of digestate, site average nitrogen leaching ranged from 3.41 to 99.08 $kg N ha^{-1} yr^{-1}$ and had a median value of 30.35 $kg N ha^{-1} yr^{-1}$. The average leaching for each site under the conditions of scenario FM1 and FD1 are shown in Figures 14a and 13b, respectively. I then evacuated the total nitrogen lost through leaching across the corn and soybean area within the biodigester radius.

I found that when manure was replaced with an equivalent amount of digestate the land experiencing leaching rates greater than 60 $kg N ha^{-1} yr^{-1}$ decreased from 29% to 25%. While the impact of replacing digestate with manure varied between sites, the total nitrogen lost across the simulated area increased from 46.77 to 49.42 $kt N yr^{-1}$ when digestate was applied. This shows that when manure was replaced with an equivalent amount of diestate the nitrogen lost by leaching increased. This is consistent with the findings of field based studies which have shown, at the site scale, digestates can lead to increased nitrogen leaching losses when compared to untreated manures (Nicholson et al., 2017; Schwager et al., 2016). The authors of an Ontario based field study which found increased nitrogen leaching when replacing manure with digestate

hypothesized that a contributing factor to this finding was the lower dry matter content of the digestate used (Schwager et al., 2016). The lower dry matter content of the digestate samples was a consistent factor in this work.

Scenario FM1 explored the one-to-one replacement of manure with digestate. This is consistent with how many field-based studies evaluate the environmental burden of digestate. However, this evaluation does not account for the way in which a centralized biodigester interacts with the landscape. To evaluate this interaction, I explored the case where digestate is redistributed from the centralized biodigester evenly to all agricultural land within 100 km, using scenario FD2. Under this distribution pattern, the total nitrogen applied at each site varied between 234.93 and 254.53 $kg\ N\ ha^{-1}yr^{-1}$, with 74.63 $kg\ N\ ha^{-1}yr^{-1}$ of the total nitrogen applied from digestate. The average nitrogen leaching across sites varied from 5.07 to 80.01 $kg\ N\ ha^{-1}yr^{-1}$, with a median value of 32.95 $kg\ N\ ha^{-1}yr^{-1}$. The distribution of site average leaching rates is shown in figure 14c. Under the conditions of scenario FD2, the total nitrogen lost by leaching across the biodigester radius from corn and soybean cropland was reduced to 43.42 $kt\ N\ yr^{-1}$. When digestate was distributed according to FD2, only 9% of the land in the biodigester radius exhibited leaching rates above 60 $kg\ N\ ha^{-1}yr^{-1}$. This shows that when considered at a regional scale, the replacement of manure with digestate can reduce instances of high nitrogen leaching rates as well as reduce the total amount of nitrogen lost through leaching over the region.

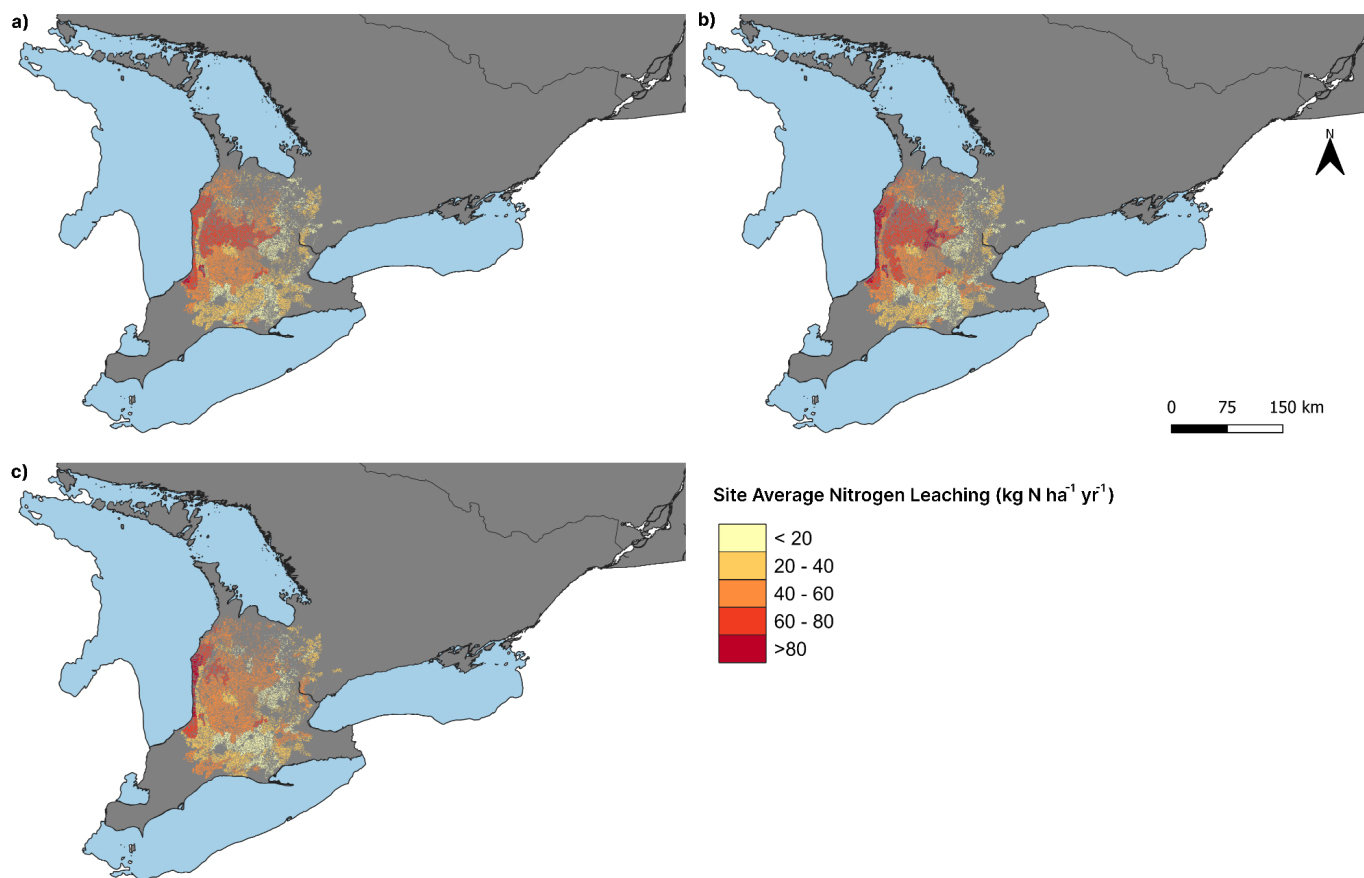


Figure 14: Average nitrogen leaching rate by site for biodigester scenarios. (a) Manure spread evenly to 75% of the agricultural land at each site, (b) digestate spread evenly to 75% of the agricultural land at each site, and (c) digestate spread evenly to all agricultural land within the biodigester radius.

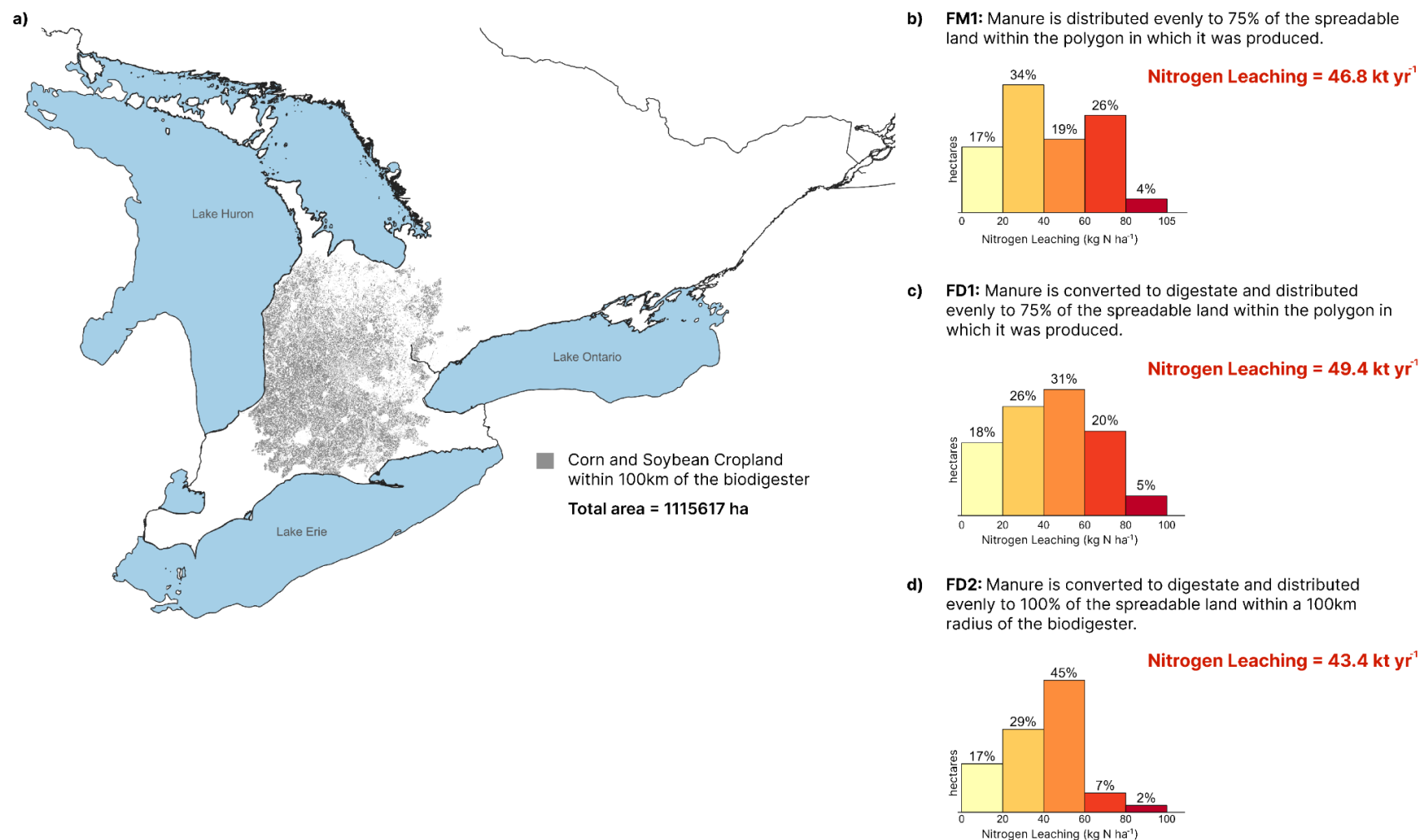


Figure 15: Annual nitrogen leaching losses from biodigester scenarios. (a) The corn and soybean cropland within 100km of a theoretical biodigester location. The 11-year average annual nitrogen losses from leaching and nitrogen leaching rate distribution per hectare of simulated land with (b) manure application under the conditions of FM1, (c) digestate application under the conditions of FD1, and (d) digestate application under the conditions of FD2.

Chapter 5 – Conclusion

This work aimed to quantify the current nitrogen leaching losses across Ontario's corn and soybean cropland and evaluate the impact a large-scale centralized biodigester could have on these losses. To accomplish this, a DNDC model was calibrated for 263 regions across the study area. The calibrated DNDC models were able to capture the general magnitude and annual variation in reported corn and soybean over an 11-year period spanning from 2011 to 2021. The median error between simulated and observed crop yields across the 263 calibrated models was 5.8%. During model calibration, corn crops were provided with synthetic fertilizer at a rate selected by the calibration procedure. The quantity of fertilizer required to meet observed corn yields across the corn cropland in the study region was approximately 69% of the total nitrogen fertilizer purchased in Ontario in 2021 showing that corn nitrogen requirements are met solely through the application of purchased synthetic fertilizer. Thus, it could be inferred that manure applications to corn crops in Ontario are applied in excess to crop nutrient needs. The calibrated DNDC models were then used to simulate the application of manure to the landscape.

The quantity of manure available in each region was estimated using livestock population data and excretion rates. Transportation constraints were placed on the manure in each site to limit the land it could be applied to, to emulate real world conditions. When the manure was applied to 75% of the agricultural land in the site in which it was produced, the average amount of nitrogen lost by leaching across all the corn and soybean cropland modeled in this thesis was $93.22 \text{ kt N yr}^{-1}$. When manure could only be applied to 50% of the agricultural land at each site, the amount of nitrogen lost through leaching increased to $94.87 \text{ kt N yr}^{-1}$. A subset of sites in a manure hotspot was then selected to explore the impact of a centralized biodigester.

I found that when digestate was subject to the same transportation constraints as manure – 75% of the agricultural land in the site in which it was produced – and applied as a one-to-one substitute for manure, the amount of nitrogen lost by leaching increased by about 6%. However, when the distribution pattern of the digestate was altered to reflect re-distribution from a centralized biodigester and the greater distance over which digestate can be transported, the amount of nitrogen lost through leaching was reduced by approximately 7%. Further, in this case only 9% of the land in the biodigester radius exhibited leaching rates above $60 \text{ kg N ha}^{-1} \text{ yr}^{-1}$. This research

shows that when used as a direct substitute and applied at equal rates based on total nitrogen content, digestate leads to more nitrogen leaching than untreated manure. However, when the system dynamics of a biodigester are accounted for (i.e. digestate is re-distributed evenly over the contribution radius of the biodigester) agricultural nitrogen leaching losses are reduced. Due to their ability to dissipate manure hotspots, biodigesters can be utilized as a tool to improve water quality in addition to generating renewable energy. However, it is important to recognize the use of biodigesters to dissipate manure hotspots and improve water quality hinges on the voluntary participation and collaboration of a wide range of stakeholders to expand the existing agricultural biogas industry in Ontario. Agricultural innovations are an important piece of reducing water quality challenges, but concurrent social and economic developments are required for widespread water quality improvement (Meredith et al., 2022).

5.1 Future Work

While the work presented in this thesis addresses a common concern for digestate – that its use may lead to increased nitrogen leaching losses – there is also concern for the gaseous emissions that are produced during its land-application. Using the methodology presented in this work, it is possible to quantify the gaseous emissions produced by digestate application. In the future, the magnitude of GHGs produced by each of the nitrogen distribution scenarios explored in this thesis will be assessed. By quantifying the magnitude of the gaseous emissions and nitrogen leaching losses which occur as a result of manure and digestate application, the GHG emissions and water quantity benefits and tradeoffs of a biodigester can be better assessed.

Additionally, the work presented in this thesis explores the nitrogen leaching losses when digestate is applied in addition to a typical commercial fertilizer application. Since crop yields were met with the synthetic fertilizer application without requiring the nitrogen in the manure or digestate treatments, nitrogen was overapplied at all sites. Scenarios which consider digestate application in place of commercial fertilizer and digestate application with reduced commercial fertilizer application should be explored in the future to evaluate the potential commercial fertilizer offsets and crop yield impacts. As the production of commercial fertilizer is a very environmentally taxing process (Menegat et al., 2022), offsets to its use provide both economic and environmental benefits which should be assessed.

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Appendix A – Saxton Rawls Pedotransfer Functions

In this thesis, the Saxton Rawls pedotransfer functions were utilized to determine the saturated hydraulic conductivity of each soil (Saxton & Rawls, 2006). The Saxton Rawls equations define saturated hydraulic conductivity of a soil using relationships between soil texture and organic matter content (OM). The equations define a soil's texture by its clay (C) and sand (S) content. The saturated hydraulic conductivity of a soil is defined with the following equation:

$$K_s = 1930(\theta_s - \theta_{33})^{(3-\lambda)} \quad (12)$$

where K_s is saturated hydraulic conductivity [$mm\ h^{-1}$], θ_{33} is the field capacity or moisture content at 33 kPa (%v) as defined by equation 13, θ_s is the moisture content at saturation (%v) as defined by equation 14, and λ is the slope of the logarithmic tension-moisture curve as defined by equation 15.

$$\theta_{33} = \theta_{33t} + [1.283(\theta_{33t})^2 - 0.374(\theta_{33t}) - 0.015] \quad (13a)$$

$$\theta_{33t} = -0.251S + 0.195C + 0.011OM + 0.006(S * OM) - 0.027(C * OM) - 0.452(S * C) + 0.299 \quad (13b)$$

where θ_{33t} is the intermediate field capacity (%v), C is clay content (%w), S is sand content (%w), and OM is organic matter content (%w).

$$\theta_s = \theta_{33} + \theta_{(s-33)} - 0.097S + 0.43 \quad (14a)$$

$$\theta_{(s-33)} = \theta_{(s-33)t} + (0.636\theta_{(s-33)t} - 0.107) \quad (14b)$$

$$\theta_{(s-33)t} = 0.278S + 0.034C + 0.022OM - 0.018(S * OM) - 0.027(C * OM) - 0.584(S * C) + 0.078 \quad (14c)$$

where $\theta_{(s-33)}$ is saturated moisture content minus field capacity (%v) and $\theta_{(s-33)t}$ is the intermediate saturated moisture content minus field capacity (%v).

$$\lambda = 1/B \quad (15)$$

where B is the coefficient of moisture tension and is defined by equation 16.

$$B = [\ln(1500) + \ln(33)] / [\ln(\theta_{33}) - \ln(\theta_{1500})] \quad (16)$$

where θ_{1500} is the wilting point or moisture content at 1500 kPa (%v) and defined by equation 17.

$$\theta_{1500} = \theta_{1500t} + (0.14 * \theta_{1500t} - 0.02) \quad (17a)$$

$$\theta_{1500t} = -0.024S + 0.487C + 0.006OM + 0.005(S * OM) - 0.013(C * OM) + 0.068(S * C) + 0.013 \quad (17a)$$

where θ_{1500t} is the intermediate wilting point (%v).

While pedotransfer functions can aid in determining missing or inaccurate hydraulic properties of a soil, it is important to note that there is uncertainty associated with their use. The associated uncertainties for the Saxton-Rawls pedotransfer functions used are listed in Supplemental Table A1 (Saxton & Rawls, 2006).

Supplemental Table A1: Saxton-Rawls pedotransfer uncertainties.

Property	Coefficient of determination (R^2)	Standard error of estimate (S_e)
θ_s	0.29	0.04
θ_{33}	0.63	0.05
$\theta_{(s-33)}$	0.36	0.06
θ_{1500}	0.86	0.02

Appendix B – Synthetic Fertilizer Application Rate Estimation

Supplemental Table B1: Seeded area and synthetic fertilizer allotment by crop type. Seeded and harvested area is from the 2021 Ontario Field Crop Production dataset (OMAFRA, 2024b)

Crop Type	Area Seeded (Acres)	Area Harvested (Acres)	Estimated N Application ($kg\ ha^{-1}$)
Winter Wheat	1,187,998	1,142,713	100
Spring Wheat	113,046	113,046	100
Fall Rye	112,010	54,777	90
Oats	84,320	69,267	55
Barley	68,756	62,481	70
Mixed Grain	59,961	50,273	80
Grain Corn	2,202,465	2,184,610	-
Canola	43,079	41,767	100
Soybeans	2,806,255	2,800,642	0
Dry White Beans	56,340	56,176	0
Colored Beans	74,412	70,248	0
Fodder Corn	289,678	272,403	-
Hay	1,719,408	1,668,288	30

Appendix C – Average Manure and Digestate Properties

Supplemental Table C1: Average manure properties by livestock type. The average manure properties as reported in the AgriSuite Organic Amendment 2024 databank (OMAFRA, 2024a). Broilers and Chickens are grouped together in the reporting of manure properties.

Type	Form	Samples	N_{total}	NH_4	NH_4	DM	C:N	pH
			%wb	%wb	% N_{total}	%wb		
Beef	Solid	1186	0.87	0.15	17.24	31.87	15.46	7.9
	Liquid	353	0.37	0.13	35.14	8.80	11.67	7.1
	Weighted Average				21.35	26.58	14.59	7.7
Dairy	Solid	721	0.64	0.11	17.19	30.84	35.02	7.9
	Liquid	3753	0.34	0.14	41.18	7.82	9.95	7.2
	Weighted Average				37.31	11.53	13.99	7.3
Hogs	Solid	138	0.88	0.23	26.14	30.16	13.83	6.6
	Liquid	3981	0.38	0.25	65.79	3.39	2.61	7.6
	Weighted Average				64.46	4.29	2.99	7.6
Chickens	Solid	2706	2.77	0.52	18.77	60.15	7.06	7.7
	Liquid	217	0.78	0.53	67.95	9.38	3.86	6.3
	Weighted Average				22.42	56.38	6.82	7.6

Supplemental Table C2: Average anaerobic digestate properties. Average properties as reported in the AgriSuite Organic Amendment 2024 databank (OMAFRA, 2024a).

Type	Form	Samples	N_{total}	NH_4	NH_4	DM	C:N	pH
			%wb	%wb	% N_{total}	%wb		
Anaerobic Digestate	Solid	22	1.18	0.21	17.80	41.05	17.63	8.1
	Liquid	150	0.52	0.28	53.85	5.56	4.44	7.9
	Weighted Average				49.24	10.10	6.13	7.9