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Research Paper

The CIRKULÆR model – A national and regional static flow model of agricultural production, environmental and climatic impacts

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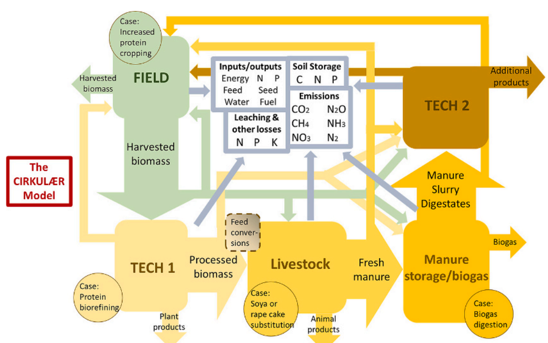
HIGHLIGHTS

- New static flow model developed for regional evaluation of agricultural systems.
- Environmental and climatic impacts from possible future scenarios of farm system changes were quantified.
- Intensive green biomass production instead of cereal cultivation increased farm-related GHG emissions.
- Return of bio refinement side streams to fields entailed CH_4, N_2O and NH_3 emissions and increased carbon storage in soils.
- Impacts from changes in organic farming were less than corresponding changes in conventional farming.

GRAPHICAL ABSTRACT



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ABSTRACT

CONTEXT: Intensive agriculture is a complex, partially industrial and partially circular system that stretches outside the boundaries of fields, herds, and farms. Increasing circularity in agriculture for both environmental and economic reasons requires ex-ante assessment tools designed to operate at the same scale and level of complexity.

OBJECTIVE: To address this, we developed the CIRKULÆR model, which evaluates system-wide climate and environmental effects of changing agricultural practices at a highly interconnected regional scale.

METHODS: The model estimates inputs, outputs, emissions and the flow of biomass, C, N, P, K and energy from crop cultivation and animal production to storage and processing of biomass. We demonstrate the capabilities of CIRKULÆR in a case study based in Denmark, which explored the substitution of cereals with protein crops followed by different storage and utilization steps. We considered twelve scenarios, each involving one of four protein crops (grass-clover, organic grass-clover, alfalfa and faba beans) in one of three soil types (coarse sand, irrigated sand and clay).

RESULTS AND CONCLUSIONS: The greatest differences from business-as-usual baseline were seen in grass-clover, organic grass clover and alfalfa scenarios. Here, biomass processing led to reduced soya imports and

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increased biogas production, an increase in direct and indirect farm-related GHG emissions and a considerable increase in soil carbon sequestration which, combined, resulted in a decrease in net farm-related GHG emissions. Finally, out-of-farm GHG emissions increased for grass-clover, while a reduction in alfalfa and faba bean was driven by lower N fertilizer imports.
SIGNIFICANCE: These findings represent valuable insights for planning future incentives and policies in agriculture. In addition, the wide range of scenarios that can be evaluated by the CIRKULÆR model underpin the potential of the model to support decision makers.

1. Introduction

Agriculture in the industrialized world is currently faced with the difficult challenge of continuing to increase food productivity, including animal production, while at the same time reducing its environmental and climate impacts, and contributing to regional and global green transitions (Schulte et al., 2019). In order to maintain or increase productivity while transitioning to more sustainable agricultural practices, particular focus is needed on increasing the circularity of agricultural systems (Velasco-Muñoz et al., 2021), thus reducing their dependency on environmentally burdensome external inputs and increasing resource use efficiency.

Circularity in this context is understood as the valorization, movement and use of plant and animal biomass primarily for food production and secondarily to produce non-food goods, all within a mixed and decentralized agricultural-industrial system. What this means is that circularity is not assumed for an individual farm but is shared between farms and other types of facilities within a local area or collection of local areas where biomass products and side-streams can be moved easily. The grain produced in one farm or field may be sold in the market or used by a different farm as feed, while the straw may be left on the fields or sold to a local power plant. In turn, livestock manure may be returned to the soil on-farm, traded with a neighboring farm, or sold to a biogas processing plant. Biogas digestate can itself be returned to the fields or can be further processed. At each step, one biomass utilization choice may entail the need to import plant nutrients, animal feed or feedstock for an industrial process from regional or global markets. The variety of valuing and utilization pathways for biomass is in fact overly complex and diverse, more so as new technologies for its use are developed. In these systems, biomass is valued by its energy content, as well as its nutrient content and its specific chemical or physical composition (e.g., biochar), where the value often transforms as the biomass itself is transformed. While this is by far not a universally useful concept of circularity, and alternative definitions abound (Kirchherr et al., 2017), it is useful in the context of regional agricultural systems, where the value of biomass and its constituents interacts complexly with the value of external inputs and product exports for a wide range of stakeholders.

Transitioning towards circular agricultural systems has numerous potential environmental and economic benefits, such as increased returns of photosynthesized carbon to the soil, leading to increased soil carbon sequestration and improved soil health (e.g., Domingo-Olivé et al. (2016); Gómez-Muñoz et al. (2021)). Likewise, promoting internal cycling of macronutrients can lead to improved farm-level use efficiency and reduced dependence on external inputs such as rock phosphate and Haber-Bosch nitrogen (Harder et al., 2021). Additionally, increased circularity can help farmers, like most businesses and industries, protect their practices from climatic, economic and geopolitical supply-chain instabilities (MacArthur, 2013). However, due to the complexity of agricultural product and by-product chains, circular agriculture policies and management recommendations envisioned with narrow goals (e.g., reducing material or energy inputs) can be less effective than intended when evaluated in a broader perspective and can lead to unexpected economic, climatic and environmental consequences (e.g., Fan et al. (2018); Kizito et al. (2019)). Thus, there is a pressing need worldwide for broad *ex-ante* sustainability assessments of circular agricultural practices for which modelling tools are uniquely suited.

Several models and frameworks have been developed which are capable of analyzing different aspects of circular practices in agriculture at different scales. For instance, Koppelmäki et al. (2021) assessed the circularity of agri-food systems in three regions in Finland based on regional statistics. Meanwhile, van Selm et al. (2024) implemented the FOODSOM model at the national scale to evaluate the effects of circular practices and dietary changes in the Netherlands on GHG emissions and land use. At continental scale, van Zanten et al. (2023) and Billen et al. (2021) have calculated the effects of circularity in agri-food systems, respectively on GHG emissions and the N cycle, across Europe. Finally, several models exist that can evaluate the economic response of farming systems to policy changes promoting circularity (see Rizojeva-Silava et al. (2018); van der Linden et al. (2020) for a few key examples, including the EU's CAPRI model).

In this study, we present here the CIRKULÆR model, a static flow model capable of capturing complex biomass, nutrient, and energy flows within and between farms and farm-related industries involving a wide variety of crops, farming practices and processing technologies. The focus of the CIRKULÆR model is to compare resource utilization and environmental impacts between scenarios by explicitly calculating and balancing biomass, element, and energy flows from primary production to livestock to industrial processes. The CIRKULÆR model is set apart from many of its relatives by operating flexibly at scales ranging from a collection of neighboring farms to a region or country and by its detailed description of flows, inputs, outputs and emissions. The principal objective of CIRKULÆR is to inform policymakers and other stakeholders early in the process of developing new regulations and incentive schemes. Thus, CIRKULÆR is designed to be as broad and comprehensive as possible regarding the different material and energy streams and transformations potentially present in a complex, partially circular agricultural system, as well as the related climate and nutrient emissions (ranging from, e.g., different crops and animal species to multiple stabling configurations, processing technologies and biomass storage practices). Finally, the model assumptions and parametrization are fully accessible, where hundreds of details can be reviewed and manipulated by the user to suit their concrete scenarios of interest (e.g., average grain yield, methane leakage rates in biogas digestor facilities, or the ammonia emission per year-dairy cow heavy breed in different types of stable).

In addition to describing CIRKULÆR, we demonstrate the model's implementation and capabilities via a case study developed as part of a policy support task for the Ministry of Food, Agriculture and Fisheries of Denmark. This case study consisted of twelve scenarios evaluating the effects of increased plant protein production in different soil classes on GHG and nutrient emissions, food production, feed imports and energy production, relative to current crop and animal production in Denmark.

2. Methods

2.1. Model overview

The CIRKULÆR model is a static-flow mass and energy transfer model for calculating emissions (N, P and K surplus/leaching, GHG emissions) as well as biomass, element (C, N, P and K) and energy (E_{bio}) balances in agricultural systems. The CIRKULÆR model tracks these mass and E_{bio} flows step-by-step through cropping, livestock, and processing technologies such as oil pressing, biogas production, pyrolysis, and protein bio-refining, as well as intermediate storage and biomass returns to the soil.

The time-step of the CIRKULÆR model is one generic farming year (i.e., between consecutive sowings in spring, no weather data input) representing present climate and technological conditions, while the areal unit is one hectare of a given soil texture class. The intended spatial scale is primarily regional with an upper limit at the national level and lower limit at an assembly of local farms and processing plants. A fundamental assumption of CIRKULÆR is that the agricultural system is constant over time, i.e., with no temporal variation in the areal distribution of crop species on soil types, as well as the number or distribution of stabled livestock species or types, or handling of resulting biomass streams. This, in turn, entails several further assumptions: that fertilizer requirements, type and application methods are fixed, the required amount of fodder for livestock is met every year (feed stocks are not tracked from one year to another and excess fodder is returned to the field), and, finally, that C deposition rates from crops and manures are constant, allowing for calculations of changes in soil C stocks between different scenarios.

The CIRKULÆR model is highly dependent on large-scale parameters such as emission factors and yearly crop productivity, which are naturally subject to change and refinement. Additionally, CIRKULÆR calculates fluxes and emissions distributed over many physical sources, both point and diffuse, many of which are not directly measurable (e.g., N_2O emissions over a regional production chain). This means that "ground-truth" datasets are not available and model validation or evaluation in the conventional sense is not possible. Thus, CIRKULÆR is not meant to produce accurate stand-alone predictions of emissions, productivity, or input requirements in a given system. Instead, the model is meant to be used for comparing scenarios of interest against a given reference scenario based on real-world statistics, with concrete differences in the form of different cropped areas, herds of varying sizes and species, different biomass storage and processing technologies and different choices of consumables at each step. In turn, the model provides system-wide calculations of inputs, outputs and emissions that can be compared between the scenarios, usually relative to a form of "business-as-usual". A key principle for scenario comparisons is keeping other parts of the model equal across scenarios in order to observe the effects of interest throughout the system unconfounded. For instance, when the differences of interest between scenarios pertain specific crops; the livestock amounts, biogas production, manure storage technologies, etc. are preserved between scenarios. However, minor additional differences in the set-up of some scenarios may need to be implemented due to cascading effects from the scenario changes (e.g., if the energy content of feed rations differs between scenarios due to changed feed production, digestion and enteric methane emissions will also slightly differ and thus also the amount of manure produced). Finally, model users have full open access to the model's parametrization tables, which contain all default partitioning, productivity, and emission factors. This allows the user to examine the quantitative assumptions and calculations behind model results in different scenarios, consider their validity in context and make informed, nuanced judgements based on the modelled differences.

The tables containing the full parametrizations of all default crops, animals, storage methods and processing technologies are publicly available on GitHub (https://github.com/JorgeMirandaVelez/CIRKULAER-model), together with supporting documentation.

2.2. Model structure

The CIRKULÆR model is divided into five modules, each handling a step in the production-processing-storage-utilization cycle of biomass in an agricultural system (Fig. 1). The modules follow the sequence: crop cultivation (Field), initial biomass processing (Tech 1), animal production (Livestock), manure storage and biogas digestion (Storage/Biogas),

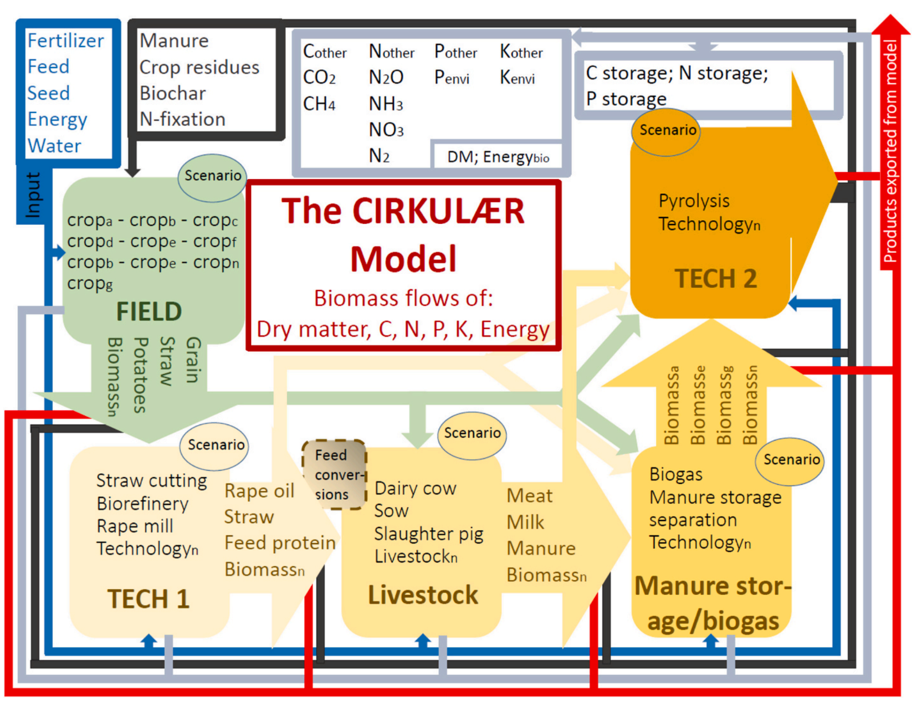

Fig. 1. Overview of the CIRKULÆR model. The modules that make up the model (Field, Tech 1, Livestock, Storage/biogas, and Tech 2) are shown in the sequential order of the calculations. Each module has different parameters connected to it in the associated scenario files, e.g., cropping area and crops in the field module, the number of livestock species in the Livestock scenario and biomass flows into various technologies/storage facilities in the Tech and Manure storage/biogas modules. The listed losses in the upper center grey box with the suffix 'other' constitute flow paths that have no consequences for climate or environment (e.g., N_2 (denitrification) and CO_2 from livestock respiration (due to climate neutrality), but still need to be tracked to fulfill the requirement of mass balance throughout the model. K_{envi} and P_{envi} correspond, respectively, to surpluses/losses of potassium and phosphorous in the fields or to the surrounding environment.

and an additional processing module to treat digested products and leftover biomass pools (Tech 2).

Each module consists of a spreadsheet book with several standardized sheets (Index Cards) with the full parametrization of crops, livestock species, and processing technologies within the model. For instance, the book associated with the Field module contains a series of Index Cards that define each crop regarding input (i.e., N, P, K irrigation water, seed, and diesel consumption), yields and biological N fixation, as well as extra sheets holding information on e.g., allometric coefficients of above and belowground crop residues. These Index Cards, in combination with user-defined Scenario and Crop Sequence files, inform the specific configuration of the main production/processing/storage choices in each step. Besides different crops and livestock species, both conventional and organic practices are included for all biomass pools and processes in the Field and Livestock modules, which in turn can be included alone or in a mixture with conventional practices in a given scenario. As the biomass moves forward in the model, the model concurrently tracks the required inputs (e.g., electricity, diesel, fertilizer, feed, and water), system losses (e.g., nutrient leaching and GHG emissions), and product exports (e.g., plant or animal products, biochar) always ensuring conservation of mass, elements and E_{bio}. Biomass streams consist of different biomass products produced during the model run, e.g., pork meat, grass seed, retained straw, etc., each associated with a particular composition (dry matter content, energy, C, N, P, and K contents). These biomass types can be either defined, with fixed compositions (e.g. crops, meat and plant oil) or undefined, meaning that their composition depends on the combined composition of streams from which they are derived (e.g., biogas digestate depends on the composition of the parental material for the digester). As all input requirements are assumed to be met (i.e. crops are fertilized optimally and animals are always fed optimally), any differences between the nutrient and E_{bio} requirements in the Field and Livestock modules and nutrient and E_{bio} contents of the internal streams returning from other modules are balanced with imported consumables (e.g., mineral fertilizer, soya-based feed). Additionally, incorporation of animal manure, green manure, biochar, biological N fixation and crop residues in the soil is recorded as the biomass moves forward in the model. Crop residues comprise both returned harvested residues such as straw that is ploughed into the soil, and non-harvestable residues such as belowground residues. The recorded losses consist of biomass DM and E_{bio} loss (from conversion inefficiencies), CO_2, CH_4, N_2O, NH_3 and N_2 emissions, NO_3^- and P leaching, and other undefined C, N, P and K losses. Table 1 presents an overview of the main parameter sources for biomass production, required inputs, utilization efficiency and emissions calculations that make up the model. Sources for all individual parameters and factors are included in the parametrization tables available online.

Finally, the model calculates C, N, P and K balances in soil per hectare. These balances are calculated between the respective element contents in fertilization, soil organic matter C turnover with fixed C-to-N ratio, crop N, P and K utilization, and, finally, the element contents of biomass returned to the soil. Each module produces a complete inventory of all biomass pools as well as total inputs and losses, which updates the output inventory of the preceding module.

The backbone of the C turnover and storage calculations in CIRKULÆR is the division of C into five categories, namely plant C, manure C, digested plant C, digested manure C, and biochar. The history of biomass C in terms of processing or bioeconomy conversion has been found to influence the degradation time in soil, which is therefore assumed to differ between different C pools in CIRKULÆR (Andrade Díaz et al., 2024; Thomsen et al., 2013). The biochar C turnover will be treated separately (not relevant for the present study case) as a two-compartment model as suggested by Andrade Díaz et al. (2024), among others. The turnover of the four non-biochar C pools is based on the C-tool model (Taghizadeh-Toosi et al., 2014), which calculates the decomposition and translocation of crop residue and manure C, and which was modified to further include digested plant and manure C by using parameters suggested by Hansen et al. (2020).

Table 1
Overview of the sources for main default model parameter data.

Data category	Description	Source
Crop yields	Provides default yields for crops in Denmark dependent on six soil classes	Mfvm (2020)
Straw and residues	Coefficients for straw and crop residues relative to harvested yields	Taghizadeh-Toosi et al. (2014)
Fertilizer amounts	Provides the default N, P and K requirements for crops in Denmark as well as interactions between crops regarding nutrients, e.g., legacy effects	Mfvm (2019, 2020)
Diesel consumption	Provides default diesel consumption for field operations	Dalgaard et al. (2002)
Livestock feed rations	Default dry matter, N and P contents in livestock feed rations	Børsting et al. (2021)
Livestock meat production	Growth and nutrient content of meat at different life stages.	Børsting et al. (2021); Mai-Lis Andersen et al. (2021)
Livestock stables	Default bedding quantities, N emissions and DM manure losses from stabling systems	Børsting et al. (2021)
Methane emissions	Methane emissions from manure in stables and storage facilities	IPCC (2006); Nielsen et al. (2023)
Losses/emissions from manure storage and field application of fertilizers	Provides the average application methods for organic fertilizers and the associated ammonia losses as well as the average ammonia emissions from mineral fertilizers. Also lists ammonia and nitrous oxide emissions from manure storage.	Nielsen et al. (2023)

2.3. Model operation

The executing part of the model is written in the R programming language (R.CoreTeam, 2022), Index Cards, Scenario files and Crop Sequence files are compiled into Microsoft Excel books.

Generally, a series of R scripts read and write a set of sheets, performing calculations, updating the model variables, calling subsequent R scripts, and finally producing output files (Fig. 2). After initializing the model with parameters from the chosen index cards, a crop sequence file (in the Field module only) and a scenario file are produced (in each of the modules), where the user can specify the areal distribution of crops, housing systems, number and species distribution of livestock and the technologies to be used in biomass storage and processing. The model then performs all production, partitioning, transfer, export, and losses calculations, as well as the energy and nutrient balances of the system, which are written in an output file.

An overall rule for products in the CIRKULÆR model is that the hierarchy of naming follows the template: Product name, Biomass pool name, Product group name, and Destination group name. All products are defined according to contents of DM, C, N, P, K and E_{bio} on the Product name level, however, when a module is completed, all products are summed on Biomass pool level and the declarations for the Biomass pools are calculated as the weighted average of the comprised products. This procedure ensures that a wide range of specific crop or livestock species can be included simultaneously while the number of biomass pools are kept minimal (e.g., several cereal crops are grown, but there is only one pool for the resulting cereal straw and one for the grain). These and other model terms are provided with a definition in Table 2. Below,

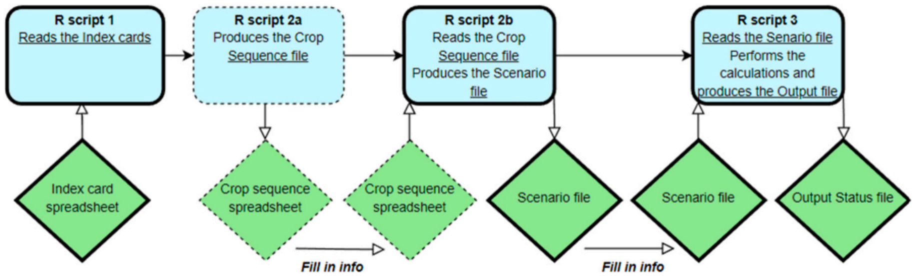

Fig. 2. The principle of operation of the CIRKULÆR model modules, consisting of R scripts (squares) and spreadsheets (diamonds). The general principle is outlined in bold black line, indicating reading information from parameter sheets (upward open arrows), writing new sheets (downward open arrows), internal data transfer between scripts (horizontal closed arrows) and capture by the user (horizontal open arrows).

Table 2
Overview of terms in the circular model.

Term	Definition
Product	The lowest level of definition of a product
Biomass pool	The name of a merged pool of more products
Product group	A suffix with a specific meaning attached to a biomass pool
Destination group	A suffix with a specific meaning attached to a biomass pool
Module	A block in the model design that produces a total inventory of biomass pools, inputs, and losses, when completed.
Index card	A structured spreadsheet containing info that defines an entry to the model, e.g., a crop or technology.
_conv	Suffix that indicates a conventional product/biomass pool, etc.
_org	Suffix that indicates an organic product/biomass pool, etc.
Scenario file	A spreadsheet associated with a module in which the distribution of e.g., the crops or livestock species defined in the respective index cards, or the amount of biomass that enter specific technologies, are filled in.

module descriptions are accompanied by references to specific spreadsheet books and/or tables in the online documentation. In addition, a spreadsheet book with general assumptions is available online (Book 01).

2.4. Modules

2.4.1. Field

The Field module calculates the production in the cropping area of an agricultural system, e.g., winter wheat, spring barley, a specific permanent grass crop, etc. The scenario file associated with the Field module is used to define the area of crops or crop sequences distributed among six soil types and either conventional or organic systems. CIRKULÆR assumes by default that all crops have yields and N, P and K fertilization requirements equal to those published in the Danish fertilizer norms (Mfvm, 2019, 2020) for six distinct classes in the Danish soil texture typology (Madsen et al., 1992). Thus, the model calculates total crop production and N, P and K utilization based on the area of each soil class sown with each crop as defined by the user. In the case of organic cropping, organic manure produced in the subsequent modules is used as primary source. If the manures from organic sources are insufficient to cover fertilizer needs for organic cropping, the deficit is covered with conventional manures. Irrigation requirements, seeding amount, and field operation parameters are based on private advisory recommendations (SEGES, 2022), whereas diesel consumption during field operations is based on Dalgaard et al. (2002). For legumes and mixed legumes/non legumes, the biological N fixation is calculated as described in Appendix 1 (supplementary material), which consists primarily of the equation used by Høgh-Jensen et al. (2004) modified in accordance with the Styr-N project (Rasmussen, 2021). Biomass return from straw (when relevant) and other residues (i.e., belowground including root exudates and aboveground residues) are calculated from crop yields and allometric partitioning coefficients (e.g., harvest index) used by Taghizadeh-Toosi et al. (2014), while the N content of residues is derived using coefficients published by the IPCC (2019). Crop biomass contents of crude protein (CP), P, K and energy are based on data from NorFor (2020), while CP:N ratio and total carbon fraction are assumed to be 6.25 and 450 g C kg^{-1} DM, respectively, for all crops. Organic yields and N fertilizer input are adjusted relative to conventional levels according to ICROFS (2008) and Olesen et al., 2020a. The above describes the standard data sources, however, given the necessary documentation is available, additional crops can be implemented by defining their yield, fertilizer input, response irrigation, required field operations, yield protein content, etc.

Due to interactions between certain crops, the possibility to define crop sequences (e.g., rotations) was included in CIRKULÆR. This ensures, for instance, that grass in rotation is always initiated by the establishment of grass, typically under-sown in spring barley. Additionally, the Danish fertilizer legislation prescribes certain modifications to fertilizer N application based on previous crops (e.g., N application to grain crops following a legume crop needs to be reduced), which is also addressed by having crops in sequences. Crop sequences are defined by the user in the Crop sequence spreadsheet (Fig. 2), by providing a name for the sequence and then choosing up to six crops from the book containing crop index cards (as described in section 2.1). If e.g., a four-crop sequence is defined, then the model treats 1 ha of this sequence as ¼ of a hectare of each of those crops, meaning that all stages in the crop rotation are present in equal proportions at any given time. Crops without interactions are put individually (without being part of a sequence) in the scenario file. All crops and crop parameters available for the Field module are compiled in the online documentation (Book 02, one crop per spreadsheet).

2.4.2. Tech 1

The Tech 1 module receives biomass produced in the Field module as input and calculates processing according to various technologies. These technologies are defined on the corresponding index cards as the allocation of mass and C, N, P, K and E_{bio} contents from the input biomass to one or more output products, as well as any losses from the system. Additionally, the module calculates the associated energy and water consumption for the process. Alternatively, some or all biomass from the Field module can bypass the Tech 1 module.

As an example, the allocation of oilseed rape into rapeseed oil and rapeseed cake (and an associated loss) is conducted by partitioning the input biomass into the output products (rapeseed oil and cake) and losses. Here, a fixed proportion of the input biomass and C, N, P, K and E_{bio} contents is assigned to the rapeseed oil as a defined product, based on the oil's fixed composition and energy content. Afterwards, the remaining input biomass is divided between cake and loss as undefined products by fixed percentages, whose composition is allowed to change based on the input's E_{bio} and element contents. The scenario file associated with Tech 1 defines how much mass of each input biomass pool is treated by each of the technologies present in the Tech 1 module. All technologies and relevant parameters available for the Tech 1 and Tech

2 modules can be found in the online documentation (Book 03, one technology per spreadsheet).

Accordingly, the biorefinery technology (Extrac_ProteinGrassclover_conv) applied in the conventional scenarios with green biomass crops in the case study (section 3) allocates the input green biomass into four outputs: white protein (aimed for human consumption), protein concentrate (aimed for feed), pulp (aimed for biogas), and brown juice. For N, the proportional allocation between the four products is 0.0128, 0.5459, 0.3707, and 0.0706 respectively resulting in a crude protein content (g) per kg DM of 589, 605, 97, and 100.

Further technologies can be added to CIRKULÆR in the future, including by recommendation from users, provided that documentation of all input and output streams, as well as energy and water consumption, and necessary conditions for operation is available and public. Adding a new processing technology to modules Tech 1 and Tech 2 further requires that the technology use as input a material stream produced, respectively, by an existing crop in the Field module, or by an existing livestock species, storage method or previous processing technology in the Livestock, Storage/Biogas and Tech 1 modules.

2.4.3. Livestock

The Livestock module calculates feed use and production of animal products (e.g., meat, milk, and manure) based on the number (defined either as year-livestock, 365 feeding days, or produced livestock per year) and proportions of livestock types defined in the Scenario file. The module's associated book contains index cards (online documentation; Book 04) that define livestock species in terms of the required feed ration (divided into grain, high quality protein, other protein, straw, P as a macronutrient, etc.), produced products, as well as stabling and manure handling systems, which as a default are based on Danish norms for livestock (Børsting et al., 2021). The index cards can also include a certain proportion of feed ration from grazing activities. The Livestock module contains a feed ration adjusting function, which optimizes the amounts of grain and protein feed to match the minimum protein requirements of each livestock species herd defined in the index card, without exceeding or falling short of that livestock species' total DM requirements. In addition, it is possible to assign alternative feedstuffs to those defined in the main ration so that the function can switch from e.g., maize silage to grass silage in case the maize silage pool runs empty, which increases the model's flexibility at meeting feed demands of livestock. Finally, the adjusting function is allowed to import certain feedstuffs (not applicable for roughage) under certain conditions to match the feedstuff amounts required in each optimized ration. For instance, if there is not enough high-quality protein entering from other modules to meet the optimal protein amounts calculated by the adjusting function, soya beans are imported to cover the difference. The result is final DM biomass rations for all groups of livestock species, and associated C, N, P, K and E_{bio} flows. Hereafter, the model subtracts three categories of output and losses pools: 1) the mass and composition of produced products e.g., milk and meat (including carcasses), 2) the respiration losses, and 3) enteric methane production. The latter two are based on equations of the energy feed ration content. For pigs, the respiration is based on Thorbek et al. (1984), while cattle respiration is calculated as relative to methane production (Madsen et al., 2010). Enteric methane calculation follows the method of the Danish national emissions inventories (Nielsen et al., 2023). When these three groups of pools are subtracted from the ration content, the remaining is assigned as animal excretion (urine and feces pooled). The excretion is distributed among stabling systems and, if relevant, bedding material is added, while also considering excretions left on the field during any grazing period (the proportion of grazed feed to total feed is assumed equal to the proportion of total excretions left in the field). Manure losses from stables and field in terms of DM, CH_4, NH_3, N_2O and N_2 are calculated according to IPCC methodology (IPCC, 2006) (with modifications regarding swine and cattle slurry following Nielsen et al. (2023)) and Danish norms Børsting et al. (2021). Finally, the dry matter, C, N, P, K and E_{bio} contents are allocated according to manure types. For instance, in a combined deep litter and slatted floor stabling, the manure and added bedding material is allocated to slurry and deep litter biomass pools (default allocation is described in the Danish norms (Børsting et al., 2021)). As an additional attribute for the biomass products and biomass pools, the Plant C proportion is introduced for manure types, which describes the distribution between C that has been digested by an animal and the C from plant biomass, e.g., straw in manures containing bedding. When a manure type has been assigned a Plant C proportion in the livestock module, then this is kept fixed throughout the model and used for allocation on the field application C subgroups.

To reduce the number of biomass pools, the concept of Feedstuff Conversions was developed in the model, which comprises for instance the silage process. The concept means that losses, energy input, plastic etc. are accounted for, but only for the needed amount as defined by the final feed rations. Thus, only the needed silage will be produced and there will not be either a leftover in this pool nor a shortage, unless the parental biomass runs empty.

2.4.4. Storage/biogas

The Storage/Biogas module allows the user to define certain output biomass streams from the Field, Tech 1, and Livestock modules to be used as feedstock for biogas digestion and/or cycled back for field application as organic fertilizer, while calculating the associated storage and leakage losses and emissions. The corresponding Scenario file defines the amount of biomass from different streams entering each defined storage/biogas pathway in the module, while all remaining biomasses bypass this module. An index card defines each of the storage/biogas pathways defined in the Scenario (see online documentation; Book 05), involving some or all the following steps: 1) initial storage, 2) initial separation process, 3) storage of separation output, 4) digestion in a biogas reactor, 5) storage of digested output, 6) additional separation of digested output, and 7) storage of separated (digested) output. For instance, simple storage of cattle slurry for field use only includes step 1. Storage losses are based on IPCC methodology (IPCC, 2006), while losses from liquid organic fertilizers were calculated following the Arrhenius equation as described in Nielsen et al. (2023). Storage tank slurry input and output due to field application were simulated in order to calculate average duration and temperature for storage of cattle and swine slurry for use in Arrhenius' equation. This simulation was based on assumptions of manure application patterns across a calendar year, estimating the running amount of stored slurry, combined with monthly temperatures, for the average temperature calculation (Nielsen et al., 2023). The resulting average storage times and temperatures were, respectively, 66 days and 7.2 °C for cattle slurry, and 97 days and 8.1 °C for swine slurry, whereas the digested slurry had the same storage duration as the parent material and average temperatures of 9.3 °C for cattle slurry and 10.7 °C for swine slurry.

Biogas production emissions consist mainly of methane leaks during digestion, as well as storage and transport of the biogas product. The leakage losses during digestion are set as a percentage of the biogas production by the user, with an default value of 1 % based on Olesen et al., 2020b. Since the uses of biogas are diverse and many take place outside the agricultural sector (e.g., power generation in the national grid), biogas production output in CIRKULÆR is given as an amount of produced MJ without further assumptions on how it is utilized, or whether other energy sources are substituted.

2.4.5. Tech 2

The Tech 2 module is functionally identical to Tech 1, providing the option to process unused biomass flows from the Field and Livestock modules, as well as side streams from all previous modules and output biomass from the Storage/Biogas module not returned to the field as manure. The Tech 2 module can use some or all the technologies available to the Tech 1 module, if indicated on the technology spreadsheets.

2.4.6. Final model information output

Following the execution of all modules, the import of N, P and K from commercial fertilizers is calculated as the difference between fertilization needs from the Field module and the nutrient content in the manures and biogas digestate returned from the Livestock and Storage modules, respectively. When simulating the field application of N in organic fertilizers, a field utilization efficiency percentage < 100 % is applied to their N content, following the current Danish legislation for calculating N application quotas (Mfvm, 2020). This means, for instance, that 100 kg of applied total N in cattle slurry replaces only 75 kg of mineral fertilizer. Thus, the net applied amount of total N is larger than the optimal crop requirement when the N fertilizer is (fully or partly) organic manure. This field utilization efficiency should, however, not be confused with the N use efficiency, which in CIRKULÆR is determined by the crop and soil type and thus is fully contained in the crop N requirements.

Based on the calculated distribution of N fertilizer sources, N losses in terms of N_2O and N_2 are calculated using emission factors (IPCC, 2006) and fixed ratios between N_2O and N_2 that takes soil type into consideration (Vinther and Hansen, 2004). NH_3 emissions are calculated using fixed factors by fertilizer types and an additional loss by crop type. The resulting output is a balance between the input of N, P and K from fertilizers and other amendments, atmospheric deposition and biological fixation, gaseous losses and the N, P and K content of harvested biomasses. The model then calculates the amount of N immobilized as SOM based on the estimated sequestered C in a 20-year perspective (described below) and a stoichiometric C:N ratio of 10. The remaining N surplus is assumed to be leached as NO_3^-.

The final output contains a status of Biomass pools and summed emissions and other losses, which balances the output from the Field module with addition of the imported feed in the Livestock module.

CIRKULÆR calculates an inventory of total C inputs to the soil, which are pooled into five categories: plant C (non-fed and non-biogas digested C), manure C (fed but non-biogas digested C), digested plant C (non-fed C), digested manure C and biochar C. From the first four categories, a total 20-year soil C sequestration value for the scenario is calculated based on the C input in each category and category-specific sequestration potential factors. These factors are calculated outside of CIRKULÆR using the C-TOOL model as described in Appendix 2 in the supplementary material. Finally, biochar degradation (not relevant for the included case), as well as corresponding C sequestration potential and GHG emissions are calculated separately.

The resulting GHG emissions calculated by the model for a given scenario can be divided into farm-related and out-of-farm emissions. A major part of the emissions sources included are counted as farm-related, including energy use at farm, for field operations or electricity use in stables. The predominant three categories of out-of-farm emissions are energy consumption that does not take place on the farms, e.g., energy use for processing at a potato factory or truck transportation of processed feedstuffs, methane leakage at the biogas plants (since biogas production is not considered a part of the agricultural sector), and emissions related to production/mining, transportation etc. of mineral fertilizers.

2.5. Internal model validation

To ensure the internal consistency of model's calculations, a scenario representing all agricultural production in Denmark in 2021 was run, and model outputs were compared with available figures, e.g. from Statistics Denmark Statbank (Statistics Denmark, 2023). The main outputs evaluated during model validation were crop production, livestock production, imports/exports, GHG emissions, applied organic fertilizers and ammonia emissions. Whenever model output differed from available statistics, the associated sequence of calculations was revised to correct calculation and programming errors, and otherwise unexplained deviations were investigated via expert opinion.

3. Case study

This case study is part of a larger assessment carried out by the Department of Agroecology at Aarhus University under request from the Ministry of Food, Agriculture and Fisheries of Denmark in 2024 (Thers et al., 2024). In the original assessment, a large set of case scenarios for increased plant protein production in Denmark were analyzed using the CIRKULÆR model, including a wide range of protein crops, conventional and organic practices and all soil texture classes in the Danish soil typology (Adhikari et al., 2013).

In the present case study, we consider twelve increased plant protein production scenarios, created by substituting 1000 ha of cereal production in one of three soil texture classes in Denmark with one of four protein crops, respectively. This arbitrary substitution area was chosen to ensure field production was sufficiently large for conversion into unitary inputs in other modules (e.g., feed for a single animal unit), while not surpassing the total area of cereal production in any soil type in Denmark (list of cereal areas on relevant soil types and the national total in appendix 3 (Table S8). The baseline scenario consists of the existing agricultural system in Denmark at national scale circa 2020 in respect of crops, livestock and biomass flows for biogas, straw-based heating facilities, processing of sugar beets and potatoes etc. Crop distribution was the average of reported field-scale crop-types from 2018 to 2022 by the Agricultural agency (DAA, 2023). All model results are presented as changes in inputs, outputs and emissions relative to baseline, normalized per hectare of substituted cereal cropping area (Baseline results in absolute figures are presented in Appendix 3). Output products from the model that are not utilized in the model, are listed in the final output as vacant for exports or other purposes outside the agricultural sector. For instance, for cereals, the final output shows the quantity that was not used for feed in Denmark.

The three soil texture classes consist of a) coarse sandy soils (< 10 % clay), b) sandy soils (< 10 % clay) with irrigation and c) clayey soils (15–100 % clay) (Appendix 4). These represent the dominant soil types and texture-dependent irrigation practices in Denmark. The protein crops considered here consisted of 1) conventional grass-clover, 2) organic grass-clover ("Økologisk" system in Denmark, Landbrugsstyrelsen (2022)), 3) conventional alfalfa and 4) conventional faba bean grown to maturity. In each scenario, the proportions between cereal species substituted with protein crops followed that of the baseline scenario in the given soil type.

The four protein crops represent three functionally different alternatives for increased plant protein production in Denmark. Grass-clover, both conventional and organic, represents a high-yielding N fertilized green biomass crop for protein biorefining, alfalfa represents a high-yielding N-fixing green biomass crop for protein biorefining and, finally, faba beans represent pulses for direct use as animal feed. Consequently, the different protein crops follow distinct processing and utilization pathways after harvest. Grass-clover and alfalfa biomass are transferred directly to the protein biorefinery (see the Tech1 section 2.4.2). The pulp fraction exiting the biorefinery is then digested for biogas, transferred to a storage tank, and finally applied to the field as green manure. The brown juice side-stream from the biorefinery is applied to the field undigested. Most of the protein produced in the biorefinery is used as feed for livestock (considered as soya-quality), although a small fraction of the extracted protein is considered for human consumption (white protein). In contrast, faba beans grown until maturity are used directly as feed for livestock (considered rape-cake-quality) and are not assumed here to produce any green biomass for processing or protein for human consumption. Yields for the three green biomass crops were adjusted upwards in order to reflect future improved varieties (Olsen et al., 2024), namely 20 %, 10 % and 7.5 % for conventional grass-clover, organic grass-clover and lucerne, respectively. Assumed input, yields, and contents of the crop alternatives are detailed in Table 3 and Table 4.

Additionally, the different crops were also assumed to be grown as

Table 3
Scenarios for increased plant protein production; assumed yields, fertilizer inputs, biological N fixation rates and diesel consumption during field operations. The irrigated grass-clover is applied 150 mm of water (both for the conventional and organic systems).

Case scenario	Yield	N fertilizer input	P fertilizer input	K fertilizer input	N-fixation	Diesel
	(kg DM ha^{-1})	(kg ha^{-1})	(kg ha^{-1})	(kg ha^{-1})	(kg N ha^{-1})	(Input L ha^{-1})
(1a) Grass-clover, conventional; non-irrigated coarse sand	13,390	253	34	212	135	81*
(1b) Grass-clover, conventional; irrigated sand	16,740	294	34	212	121	100*
(1c) Grass-clover, conventional; clay	14,510	267	34	212	163	87*
(2a) Grass-clover, organic; non-irrigated coarse sand	10,800	137	30	187	194	60*
(2b) Grass-clover, organic; irrigated sand	13,500	159	30	187	223	76*
(2c) Grass-clover, organic; clay	11,700	144	30	187	253	65*
(3a) Alfalfa, conventional; non-irrigated coarse sand	12,005	0	31	224	460	72
(3b) Alfalfa, conventional; irrigated sand	16,006	0	31	224	614	91
(3c) Alfalfa, conventional; clay	14,006	0	31	224	641	84
(4a) Faba beans, conventional; non-irrigated coarse sand	3910	0	32	75	195	51
(4b) Faba beans, conventional; irrigated sand	3910	0	32	75	195	51
(4c) Faba beans, conventional; clay	3910	0	32	75	209	58

* Diesel input for the grass-clover crops does not include establishment of the crop (e.g., undersown in spring barley).

Table 4
The assumed contents of carbon (C), crude protein (CP), phosphorous (P), potassium (K) and E_{bio} in the yields of crop alternatives, as well as the partitioning coefficients (a, b and c) used for calculating crop residue dry matter and N content.

Crop	C	CP	P	K	E_{bio}	a[a]	b[a]	c[a]	Residue N
	(g kg^{-1} DM)	(g kg^{-1} DM)	(g kg^{-1} DM)	(g kg^{-1} DM)	(MJ kg^{-1} DM)				(g N kg^{-1} DM)
Grass-clover	450	157	3.5	26	16.5	0.625	0.45	0	16
Alfalfa	450	184	2.8	28	18.4	0.700	0.45	0	19
Faba beans	450	287	6.1	14	19.8	0.450	0.17	0	8

[a] The coefficients a, b, and c are applied for calculating above- and below ground crop residues according to the formula: Crop residues (kg DM) = (Harvested yield (kg DM) * (1/((1-b)*a))) – Harvested yield (kg DM) – Harvested yield (kg DM)*c. In that way, firstly, the total biomass for the crop is determined and secondly, the harvested biomass and the secondary yield (straw – If any) are subtracted. The assumption is in any case 450 g C kg-1 DM.

part of different crop sequences or rotations. Grass-clover was assumed to be initially sown under a spring barley crop, grown for three consecutive years and followed by a year of spring barley. Alfalfa was assumed to be grown for three years, followed by one year of spring barley. Faba bean was assumed to be grown for a single year, followed by either a winter cereal crop (wheat or rye) or a winter cover crop and spring barley, depending on distribution between these cereals on the soil type.

Finally, global warming potentials in this case study were set as 265 and 28 for N_2O and CH_4, respectively (AR5; (Ipcc, 2013)), and the indirect N_2O emission factors from ammonia volatilization and nitrate leaching we assumed as 1 % of NH_3 N and 1.1 % for NO_3^- N (IPCC, 2019).

3.1. *Case study results and interpretation*

CIRKULÆR considers different crop properties both for baseline cereals and alternative crops depending on soil type. Thus, some of the most important differences between alternative crops and baseline such as yield, fertilizer requirements and the proportion of N surplus lost to NO_3^- leaching, varied for the same crop depending on soil type.

In scenarios involving conventional grass-clover, organic grass-clover and alfalfa, the CIRKULÆR-model estimated an increase in direct and indirect farm-related GHG emissions, as well as a considerable increase in soil carbon sequestration which, combined, resulted in a decrease in net GHG emissions, relative to baseline (Table 5, Figure 3).

Table 5
Modelled changes in GHG emissions and soil C sequestration relative to current practices in Denmark (baseline), caused by substituting 1 ha of cereal production with protein crops as defined in the twelve alternative scenarios. Positive and negative values indicating emissions/storage are, respectively, higher and lower relative to baseline. C sequestration is considered as a mitigating change in emissions in the final balance. The relative proportions of each difference of baseline values are shown in appendix 3 (Table S9).

Case scenario	Agricultural emissions					C soil storage	Balance
	Energy	Stabling and storage emissions	Emissions from fertilization, residue turnover etc.	Indirect N_2O from NO_3 leaching	Total	C storage after 20 years	Agricultural emissions including soil C storage
	(kg CO_2eq ha^{-1} y^{-1})	(kg CO_2eq ha^{-1} y^{-1})	(kg CO_2eq ha^{-1} y^{-1})	(kg CO_2eq ha^{-1} y^{-1})	(kg CO_2eq ha^{-1} y^{-1})	(kg CO_2eq ha^{-1} y^{-1})	(kg CO_2eq ha^{-1} y^{-1})
1a	221	1212	821	−570	**1683**	5648	***−3964***
1b	316	1515	1074	−993	**1912**	7344	***−5432***
1c	226	1315	672	−434	**1779**	5597	***−3818***
2a	133	894	513	−258	**1282**	4704	***−3422***
2b	170	1116	850	−450	**1686**	6143	***−4457***
2c	96	967	623	20	**1706**	4919	***−3213***
3a	166	1086	−328	−79	**845**	3891	***−3045***
3b	268	1448	−156	−47	**1513**	5683	***−4170***
3c	199	1269	−452	536	**1552**	4211	***−2660***
4a	−9	−6	−835	−286	**−1137**	−182	***−955***
4b	−9	−7	−989	−247	**−1252**	−483	***−769***
4c	−14	−5	−1127	−74	**−1220**	−971	***−249***

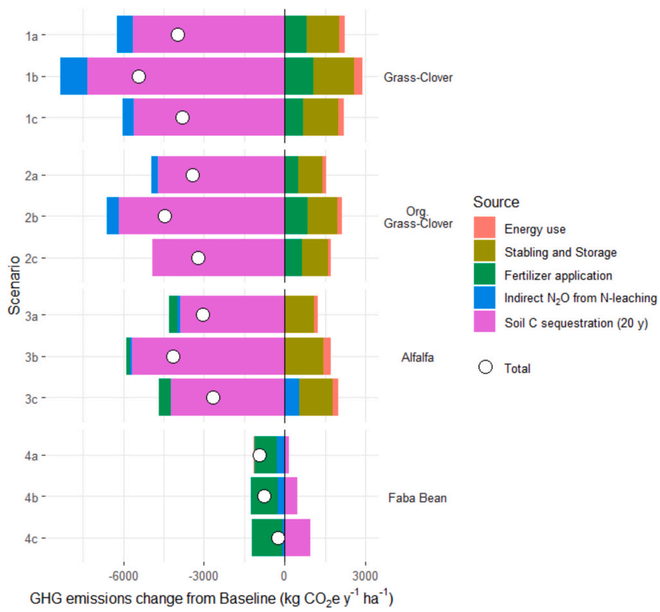

Fig. 3. Changes in farm-related GHG emissions for 12 scenarios substituting 1000 ha of cereal cropping with protein crops as calculated by the CIRKULÆR model. The changes are shown relative to a business-as-usual baseline for Denmark. Mitigated emissions are given negative values and increased emissions as positive. The white dot represents the net sum of mitigations and increases. The scenarios represent different protein crops substituting cereals in equal areas of different soil types in Denmark (Table 3).

The increases in direct GHG emissions were dominated by emissions during storage and, for clover-grass, field application of green manure side-streams from biorefining and biogas production, with a smaller contribution from increased energy use, mainly from field operations (breakdown not shown).

The considerable soil C sequestration increases calculated by the model in conventional grass-clover and alfalfa scenarios are explained by two increased soil C inputs. Firstly, increased crop residue and root exudate inputs from grass-clover and alfalfa compared to cereals. Secondly, the C input from green manure which in the model is assumed to replace mineral fertilizers with no associated C input. On the other hand, the increase in soil C sequestration was slightly lower in organic clover-grass, mainly due to lower yields leading to lower green manure production and application, as well as lower residue and root C inputs, which are calculated from yields in the model. This resulted in approximately 1000 kg CO2eq ha^{-1} y^{-1} lower total GHG savings, relative to baseline, in the organic scenarios compared to the conventional scenarios.

Parallel to increased soil C sequestration relative to baseline, returning green manure to the field in conventional grass-clover led to increases in modelled direct GHG emissions due to the substitution of mineral fertilizers with green manure, as mineral N fertilizers are not allocated direct GHG emissions during storage. This effect is compounded with the <100 % utilization efficiency of organic fertilizers implemented in the model, which applies as well to green manures and resulted in higher total N applications for equal crop N requirements, leading to even greater direct N_2O and ammonia emissions. Furthermore, ammonia emissions during application are assumed to be higher for organic fertilizers compared to mineral fertilizers, which translate into greater indirect N_2O emissions. These increases in agricultural GHG emissions were partly offset in conventional grass-clover scenarios by modelled decreases in the indirect N_2O emissions associated with N leaching, caused by soil N immobilization implicit in soil C sequestration at a 10:1 ratio, which reduced the total N surplus. The organic grass-clover scenarios, on the other hand, showed considerably lower increases in storage and fertilization GHG emissions compared to conventional management, as was the case with soil C sequestration, mainly due to lower yields and thus lower production of green manure side-streams.

The scenarios involving substitution of cereals with faba beans led to very different results compared to other alternative crops. Here, farm-related emissions were reduced by approximately 1200 kg CO_2eq ha^{-1} y^{-1}, while soil C sequestration was in fact modestly reduced, relative to baseline. Thus, among the modelled scenarios, faba beans were the alternative crop with the lowest expected reductions in net on-farm GHG emissions (between 250 and 950 kg CO_2eq ha^{-1} y^{-1}) relative to baseline. These reductions were driven primarily by low energy consumption, minimal production of green manure (and thus minimal emissions related to storage and application), and moderate reductions in secondary N_2O emissions associated with low N-leaching, given the minimal N fertilization requirements in faba beans.

CIRKULÆR also calculated other relevant environmental impacts in all twelve scenarios, including reactive nutrient emissions (Table 6). As mentioned earlier, substituting cereals with grass-clover resulted in a reduced nitrate surplus, which translates into a reduction in NO_3- lost from the rootzone through leaching. This reduction was approximately 145 and 50 kg N ha^{-1} y^{-1} in average for the conventional and organic case scenarios, respectively, although the model calculated a small increase in N leaching (4 kg N ha^{-1} y^{-1}) from organic grass-clover in clayey soils. The model also predicted an increased ammonia volatilization of 15 and 11 kg N ha^{-1} y^{-1} in average across conventional and organic case scenarios, respectively.

Imports of feed, as well as production of different feed types (Table 7), were also impacted by the cereal substitution with protein crops. Protein biorefining of grass-clover biomass led to a reduced import of protein feed, especially soya, of approximately 2800 kg and 2250 kg DM per hectare of protein crops in average for the conventional and organic case scenarios, respectively. Additionally, CIRKULÆR calculated a small production of protein suited for human consumption (Stødkilde et al., 2024) of approximately 30 kg CP ha^{-1} y^{-1} across all grass-clover scenarios and an increase in biogas production of approximately 100,000 MJ in average. Finally, grain production in these case scenarios was estimated to decrease by 5800 and 3650 kg grain DM ha^{-1} $year^{-1}$ in average across conventional and organic grass-clover scenarios, respectively.

In scenarios involving alfalfa, the model assumes slightly lower yields compared to grass-clover, which in turn led to moderately lower biogas production and a slightly reduced substitution of imported soya with biorefined protein compared with conventional grass-clover. Additionally, the model estimated modest decreases in nitrate

Table 6
Modelled changes, relative to current practices in Denmark in emissions of reactive nutrients in the 12 scenarios with increase protein crop production. The relative proportions of each difference to baseline values are shown in appendix 3 (Table S10 and S12).

Case scenario	Ammonia volatilization	Nitrate leaching	P_{emvi}	K_{envi}
	(kg N ha^{-1} y^{-1})	(kg N ha^{-1} y^{-1})	(kg P ha^{-1} y^{-1})	(kg K ha^{-1} y^{-1})
1a	14	−124	−18	−187
1b	17	−217	−26	−262
1c	13	−95	−13	−202
2a	10	−56	1	−11
2b	12	−98	−3	−28
2c	10	4	−2	−30
3a	3	−17	−11	−137
3b	6	−10	−18	−236
3c	3	117	−8	−178
4a	−7	−62	−1	−21
4b	−7	−54	2	−15
4c	−8	−16	7	−10

Table 7
Modelled changes in imports of animal fodder and production of grain and biogas after substituting 1 ha of cereal production with protein crops as outlined in the twelve alternative scenarios. The relative proportions of each difference to baseline values are shown in appendix 3 (Table S10).

Case scenario	Changed import		Changed production		
	Rape cake	Soya	Proteins for human consumption	Grain	Biogas
	(Kg DM ha^{-1} y^{-1})	(Kg DM ha^{-1} y^{-1})	(Kg CP ha^{-1} y^{-1})	(Kg DM ha^{-1} y^{-1})	(MJ ha^{-1} y^{-1})
1a	−25	−2546	32	−4603	98,299
1b	−26	−3175	39	−5700	122,892
1c	−11	2704	34	−7101	106,521
2a	−20	−2028	25	−3003	79,271
2b	−17	−2534	32	−3671	99,088
2c	16	−2187	28	−4296	85,877
3a	−8	−2783	28	−5017	88,109
3b	−8	−3703	38	−6289	117,566
3c	6	−3192	33	−7607	102,871
4a	−3363	211	0	−3093	−3
4b	−3363	210	0	−4053	−3
4c	−3350	260	0	−5358	−3

leaching in coarse sand soil types and even an increase in nitrate leaching in clay soil types under alfalfa relative to baseline. This is mainly due to the large amounts of N fixed by the crop, which increased the overall N surplus in the system and thus the assumed associated leaching.

Mature faba beans are assumed in CIRKULÆR to be comparable to rape cake feed protein and thus displaced rape cake (approx. 3400 kg DM ha^{-1} y^{-1}) instead of soya, where the model actually predicted a small increase in the import of soya relative to baseline. Similarly, the model calculated negligible changes in biogas production relative to baseline for all scenarios involving faba beans, as this crop is not expected to produce digestible biomass when grown to maturity.

The CIRKULÆR model also estimated changes in out-of-farm GHG emissions that are not typically counted as agricultural emissions (Table 8). According to the model, the scenarios involving substitution of cereals with grass-clover resulted in increased out-of-farm CO_2eq emissions, primarily associated with mineral fertilizer production. In the scenarios involving substitution with alfalfa and faba beans, on the other hand, the model calculated substantial decreases in GHG emissions related to mineral fertilizer production, as both alternative crops are assumed to be efficient N-fixers and thus require minimal N fertilization.

Table 8
Changes in the modelled out-of-farm GHG emissions for the 12 alternative crop scenarios relative to business-as-usual. Positive values mean emissions are larger compared to the base scenario. The relative proportions of each difference to baseline values are shown in appendix 3 (Table S11).

Case scenario	Sum (kg CO_2eq ha^{-1} y^{-1})	Energy use, non-agricultural (kg CO_2eq ha^{-1} y^{-1})	Leakage biogas (kg CO_2eq ha^{-1} y^{-1})	Production of fertilizer (kg CO_2eq ha^{-1} y^{-1})
1a	**1882**	1188	505	189
1b	**2253**	1485	632	136
1c	**1745**	1286	548	−89
2a	**1902**	1322	408	172
2b	**2270**	1653	510	107
2c	**1885**	1430	442	13
3a	**−167**	1010	453	−1630
3b	**−50**	1348	605	−2003
3c	**−345**	1178	529	−2052
4a	**−959**	56	0	−1015
4b	**−1079**	56	0	−1135
4c	**−1206**	54	0	−1260

Faba beans showed the largest reduction in out-of-farm GHG emissions relative to baseline; besides foregoing mineral fertilizers, the lack of biogas production entails no leakage-associated methane emissions. The lack of biogas production, besides constituting an economic disadvantage of substituting cereals with faba beans, also highlights the potential pitfall of an alternative crop that carries out only modest amounts of photosynthetic C fixing.

It is important to note that the substitution of existing energy sources with biogas produced in the different scenarios is not included in CIRKULÆR's out-of-farm GHG emission calculations. The principal reason for this is the complex coupling between energy production and consumption, which makes it impossible to make meaningful *a priori* assumptions regarding the fate of any additional biogas calculated by the model. Likewise, the decreases in protein feedstuff import and grain production calculated here have not been coupled with GHG emissions/savings, since this is also associated with cascading assumptions regarding national, regional, and global supply chains currently beyond scope for the model.

4. Discussion

The case study results presented here showed, somewhat unexpectedly, that a chain of arguably positive management choices and technological innovations, i.e. protein biorefining, energy production from residues and the circular utilization of biomass, can result in sizeable increases in on-farm GHG emissions, which potentially can be offset by long-term C sequestration. Rather than providing a final figure for the net effect of increasing plant protein production in Denmark, these results suggest that the deciding element in this balance is soil C sequestration, as is its calculation methodology.

Predicting soil C sequestration and turnover remains a difficult task, and even the most sophisticated model calculations must always be understood as narrow deterministic extrapolations beholden to sets of theoretical assumptions. Furthermore, model structures and parametrization are continuously being re-examined and improved, and as such predictions have the potential to change. Finally, when a decision is made on how to calculate soil C sequestration, further choices remain about whether and how to include this in the overall calculation of global warming impact. CIRKULÆR uses the remaining added C 20 years after application as the total soil C sequestration and equivalent CO_2eq sequestration for a given biomass stream returned to the soil. This is in line with results obtained in Denmark regarding reaching a new equilibration stage for soil C pool when changing C input management (Jensen et al., 2022a; Jensen et al., 2022b) however, these settings can be easily altered by the user depending on their approach and case-specific rationale.

In the presented version of the model, all crops are assumed to be of standard quality, meaning that no failures in feed quality were assumed. The user can define a lower quality feed or food if desired. However, the model uses defined constant DM amounts for livestock feeding and optimizes on protein content to target a predefined protein content interval for the full feed ration for each livestock species. In this way, a lower protein content in some parts of the roughage will result in a higher proportion of protein feed (e.g., rape seed cake or soya cake) in the ration.

The energy content of the ration is, however, used for enteric methane calculations. When applying solely standard quality feedstocks, the energy content of dairy cows became generally too high. Thus, the MJ content of 1 kg DM green maize whole crop was reduced by 1 MJ from 18.7 to 17.7 MJ Kg DM^{-1}, in order to consider realistic production conditions. Likewise, the energy contents of grass and grass-clover feedstocks were reduced from approximately 18.4 to 16.5 MJ Kg DM^{-1}. By introducing this change, the levels of enteric methane production from cattle became comparable to reported values, which was part of the validation process.

It is also important to point out that the livestock production across

Denmark was kept equal between baseline and all scenarios, regardless of the estimated production of protein for human consumption or the potential for substituting animal protein with plant protein. The CIRKULÆR model can in fact incorporate changes in livestock production in its scenario calculations, as well as a wide range of changes in species composition and management practices of animal production. It is therefore possible to establish scenarios that model a wide variety of dietary changes based on circularity requirements, similarly to (van Selm et al., 2024) on empirical measures such as willingness to adopt plant-based diets (e.g., (Henn et al., 2022) or on specific policy proposals. However, developing a set of concrete scenarios for dietary changes among Danish consumers given different plant protein sources considered here was beyond the scope of the present case study.

The CIRKULÆR model development was financed by the Danish Agricultural Agency with the purpose of creating a tool for carrying out general assessments of the performance and impacts of different agricultural systems. Therefore, the CIRKULÆR model has been originally developed with Danish legislation and common practices in mind, e.g., regarding fertilization rates, use and storage of organic fertilizers, herd sizes, etc. However, processes like ammonia volatilization, enteric methane production and biogas digestion, etc., are functionally similar across regions, and the flows of biomass, energy and nutrients at the regional level can be generalized to many other contexts. Thus, provided region-specific parameters such as average crop yields and soil C turnover rates are adjusted, the present model is potentially applicable to a wide range of agricultural systems outside Denmark. For instance, the trans4num project (http://trans4num.eu/en/), aiming for enhancing the nature-based solutions (NBS) implementation in Europe, is planning to include the CIRKULÆR model as part of a work package focusing on monitoring and optimizing NBS-related nutrient flows across different European regions.

In the interpretation of the case results, the produced biogas is not viewed as an agricultural output, since it was decided to follow the Danish Climate Inventory on this matter (Nielsen et al., 2023). Therefore, the methane leakage from biogas plants is not considered an agricultural emission. The choice of this interpretation is up to the user of the model.

The CIRKULÆR model has elements in common with existing farm-level models in Europe. For example, the REPRO model in Germany (Hülsbergen and Küstermann, 2006) can simulate element cycles (C, P, N and K), energy efficiency and greenhouse gas (GHG) emissions in conventional and organic crop-animal farming systems employing a few different technologies such as field operations and animal manure storage. Similarly, the FarmGHG model (Olesen et al., 2006), calculates energy needs, GHG emissions and in-farm C and N cycling in conventional and organic dairy farms in Denmark. However, the herd and farm scales are often inappropriate for analyzing circularity in agriculture, as single farms practically never act as closed systems. Importantly, some technologies key to circular resource utilization requires large economic investments and thus are frequently established as centralized facilities that can treat products and by-products from regional farmers and food industries, such as centralized biogas plants or biorefineries. Additionally, industries such as sugar factories and potato starch factories treat biomass (e.g., sugar beets or potatoes) from a large area and return some side streams to agriculture in the shape of feed or fertilizer, the latter in some cases via a biogas plant. Thus, it is a key advantage of the CIRKULÆR model that it operates at the regional and national scales, above farm level.

5. Conclusions

The CIRKULÆR model can estimate a broad range of climate and environmental effects throughout complex agricultural systems. When complemented with careful analysis of the model's cascading calculations, these estimations provide insights into both expected and unexpected effects that can otherwise be overwhelmingly cumbersome to foresee. In the case study presented here, the contribution of C soil storage to the beneficial outcome of substituting cereals with green crops for biorefinery is shown to have a decisive impact on the overall results, pointing out key considerations that must be made before expanding protein crop production in existing arable land in Denmark. In addition, a decision on inclusion of the biogas production as a negative (mitigating) greenhouse gas emission in the agricultural sector, would significantly increase the margin to cereal cultivation in terms of mitigation effect. For the seed producing alternative crop (Faba bean), the likewise inclusion of CO_2 emissions related to mineral fertilizer production (by default not viewed as an agricultural emission) would contribute to a larger greenhouse gas mitigating effect from this crop, and thus principles for system boundaries need to be addressed by decision makers.

In a broader perspective, the CIRKULÆR model represents a comprehensive support tool for management and policy decisions. This model has been developed and implemented to provide science-based policy advice in Denmark but is potentially transportable to other countries and regions. Finally, the purpose of CIRKULÆR is not to provide a final figure of the climate or environmental effects of a given practice or technology. Rather, its purpose and value lie in providing concrete quantitative comparisons between regional agricultural systems and helping identify unforeseen risks, benefits and uncertainties at the start of a policy planning process.

CRediT authorship contribution statement

Henrik Thers: Writing – review & editing, Writing – original draft, Visualization, Validation, Methodology, Formal analysis, Data curation, Conceptualization. **Lars Uldall-Jessen:** Writing – review & editing, Software, Methodology, Formal analysis, Data curation, Conceptualization. **Asbjørn Mølmer Sahlholdt:** Validation, Methodology, Data curation. **Mette Vestergaard Odgaard:** Writing – review & editing, Methodology, Data curation. **August Kau Lægsgaard Madsen:** Methodology, Data curation. **Tommy Dalgaard:** Supervision, Resources, Project administration, Funding acquisition, Conceptualization. **Troels Kristensen:** Writing – review & editing, Writing – original draft, Validation, Supervision, Resources, Project administration, Methodology, Investigation, Funding acquisition, Data curation, Conceptualization. **Jorge Federico Miranda-Vélez:** Writing – review & editing, Writing – original draft, Visualization, Supervision, Methodology, Investigation, Formal analysis.

Declaration of competing interest

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

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.agsy.2025.104415.

Data availability

Data are available online and a link is provided in the paper

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