Modelling Nutrient Flows in a Simplified Local Food-Energy-Water System

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Abstract

Sustainable use and management of nutrients is an important issue for food, energy and water systems. The close connections between the three systems, reflected by the "nexus" concept, warrant an integrated approach to nutrients management across the nexus. In this paper, dynamic modelling of nutrient flows in a local food-energy-water system is presented and applied to a simplified case study. The model was used to simulate several scenarios affecting nitrogen flows and stocks to assess the impact of a) the level of local wheat production, b) the selection of energy generation technology, and c) the management of available nutrient resources (digestate and straws). The simulation results showed that varying the proportion of locally produced wheat significantly affects the surface runoff and the nitrogen content in a local water body, with the latter increasing by nearly 70% in 50 years if about half of the wheat consumed is produced locally as opposed to being 100% imported. The introduction of anaerobic digestion as an energy generation option helps to supply more electricity, reduce the imported fertiliser, and also significantly reduce the landfilled nitrogen nutrient by up to 60 times, due to the reuse of the anaerobic digestate. On the other hand, a balanced consideration should be given between using the straw as fertiliser and as feedstock for energy generation. This work offers a first analysis of the food-energy-water nexus with a focus on nutrient flows and stocks. The modelling approach has the potential to inform holistic decision making with respect to nutrient usage, efficiency and the related environmental impact in the design of a local system for meeting the demand for food, energy and water.

Keywords: nutrients, food-energy-water nexus, recycle, local production, modelling

1. Introduction

One of the greatest challenges faced by our society today is the increasing demand for energy, food and water within a context of climate change and scarcity of resources (FAO, 2014). Food, energy and water are the three most essential needs for humans, and their natural availability and supply infrastructures can be intimately related in complex ways forming a nexus. The food-energy-water (FEW) nexus is a concept that is gaining attention to inform sustainable development strategies of a country or region, as it can potentially affect the extent to which food, energy and water security objectives are simultaneously achieved (Hoff, 2011). To tackle the complexity of the nexus, it is essential to quantify the interactions between the subsystems of the nexus and between the nexus and its environment (Chang et al., 2016). This allows for the identification of key interactions that can be manipulated to balance negative impacts currently affecting nexus resources and their provisioning systems, so that sustainable solutions can be devised (Martinez-Hernadez et al., 2017a). To-date, nexus studies have considered the global scale (Machell et al., 2015), while regional and local scale nexus studies are also needed because the impacts of nexus decisions on populations, ecosystems and activities are often localised in the first place; opportunities of making improvements also more directly call for regional and local actions (Martinez-Hernandez et al., 2017b).

As an initial step towards sustainable solutions, quantitative modelling and assessment of the nexus are required (Bazilian et al, 2011). Improving resource efficiency and environmental sustainability through (i) the integration of industrial processes and (ii) due considerations on the interactions between human activities and ecosystems has long been the central theme of industrial ecology (Allenby, 1992). Recently, assessment of the capacity of local ecosystems to meet industrial demand for ecosystem services was conducted by Gopalakrishnan et al. (2016), where synergistic techno-ecological systems operating within ecological constraints were proposed. There have been several other advances to understand and manage interactions within the FEW nexus with a focus on how to best couple the three subsystems using input-output analyses (White et al., 2017), network models (Vora et al., 2017), life cycle assessment (Irabien and Darton, 2016), mathematical modelling (Karnib, 2017)) and optimisation (Leung Pah Hang et al., 2016), insight-based methods (Leung Pah Hang et al., 2017) and other process systems engineering approaches (Garcia and You, 2016; Al-Ansari et al., 2017). A nexus simulation tool has also been developed to support the analysis of interactions between FEW components and the ecosystem at a local scale (Martinez-Hernandez et al., 2017a).

While managing nutrient flows has widely been considered in areas such as industrial ecology (e.g. in the well-known example of Kalundborg, Jacobsen, 2016) and environmental protection in coastal regions (Townsend, 1998; Howarth and Paerl, 2008), existing work on the FEW nexus has presented rather limited studies that feature an explicit analysis of nutrient flows and associated environmental impacts. Nutrients play a major role in the interconnection between food, energy, water nexus, especially affecting food and energy crop yields and also the quality of water resources (Davidson et al., 2016). In particular, the extensive use of synthetic nitrogen fertilisers has been vital for increasing the food productivity, much needed by the growing world population. However, only about half of the nitrogen fertilisers applied to farms is taken up by the crops, while the rest remains as stock in the soil or enters other parts of the environment. The latter is known to cause eutrophication of water bodies and air pollution due to the losses through surface runoff, soil leaching and volatilisation (Mortensen et al., 2016). Therefore, it is important to holistically analyse and predict nitrogen flows, which can be carried out through mathematical modelling, as demonstrated by the recent work of Singh et al. (2017) for Illinois with a focus on 3 agricultural commodities. In the context of FEW nexus, appropriate models that capture the inter-coupling between the three sectors are needed to assess different design choices, so that opportunities across the three sectors to increase resource efficiency and to reduce adverse environmental impacts can be revealed, ultimately contributing to the closed-loop management of resources (Mo and Zhang, 2013; Davis et al., 2016).

In this paper, an approach for the dynamic modelling of nutrients flows and stocks in the FEW nexus is presented via a case study based on the settings of an eco-town in the UK. The objective of the model is to simulate several scenarios which are different in the level of local wheat production, the technical options for energy generation, and the management of available nutrient resources. The simulation results are used to analyse the impact of these scenarios on imported fertiliser flows, energy production flows, nitrogen flows to landfill and air emissions, as well as the impact on water quality in terms of nitrogen concentration in a local water body. This work adopts the generic modelling approach previously proposed for local production systems (Martinez-Hernandez et al., 2017b), and has been carried out in parallel with the development of a general-purpose simulator for local food-energy-water systems (Martinez-Hernandez et al., 2017a). The unique contribution of this work lies in the detailed modelling of nutrient stocks and flows and using the model to analyse the impact of various decisions on nutrient efficiency and associated environmental aspects, including particularly those some of which could arise from the inter-coupling between the three sectors of food, energy and water. This work adopts the same case study locale as in earlier work on optimal design of local FEW systems (Leung Pah Hang et al., 2016, 2017), where cumulative exergy consumption was used as the optimisation objective. While both the exergy cost for fertilizer supply and that for reducing nutrients in wastewater to acceptable levels were considered in the optimal design work, the mathematical model used in optimisation was for steady states, therefore no system dynamics was captured. In principle, the dynamic model developed in this work can be used to support more detailed studies of the schemes recommended by optimal design, with a focus on the perspective of nutrient flows and stocks, to further inform the integrated management of local FEW systems.

2. Overall approach

The analysis of interactions between food-energy-water systems and their effects on nutrients flows and stocks in an overall local system requires a mathematical model that can capture all the important connections and dynamics. The approach followed in this work comprises the following steps:

(i) developing a conceptual description of individual subsystems and their interactions;
(ii) building mathematical models of individual subsystems;
(iii) simulating and analysing individual systems if desirable;
(iv) integration of subsystem models based on the connectivity identified in step (i);
(v) assessing the resulting nexus system through simulation studies of various scenarios of interest.

As an overview of the proposed approach, principles for developing a conceptual description (step i) and mathematical models (steps ii and iv) are presented; a detailed illustration of these steps and of the more case-specific steps for simulation and analysis (i.e. steps iii and iv) will be given through a case study in Sections 3 and 4.

2.1. Conceptual structures

A conceptual structure of a system shows the key components and connections between them. In particular, a "*source-sink*" mapping diagram can help to represent a system by showing the matches between sources and sinks. In the case of nutrient flow analysis, "sources" refer to the nutrients or material flows containing the nutrients relevant to the goals of a given study; and "sinks" refer to the processes that change or transform a nutrient flow, or the point of termination of a nutrient flow. The direction of flows, and the introduction, consumption and disposal of nutrients within or external to the system are also shown as part of the source-sink mapping diagram. The structure of a complete FEW system can be obtained by connecting the structures of individual subsystems through resource flows.

2.2. Mathematical models and implementation

From a conceptual description of a local food-energy-water system, nutrients can be identified either in *flows* between various processes such as food manufacturing, energy production and waste water treatment, or as being cumulated in soil and a water body, in the form of nutrient *stock*. The stock-flow framework enables mathematical construction of each subsystem's model. In this framework, the temporal variation of nutrient stocks is captured by differential equations that link the change in stock "levels" due to incoming and outgoing flows. These flows are determined in different ways, depending on their nature:

- For a flow representing an internal demand (e.g. bread consumption), it is typically pre-specified as part of a scenario to be studied.

- An output from an internal stock (associated with a system component) (e.g. nutrient runoff from land), which may become input to an internal process, stock or the external environment, is typically determined by solving a differential equation representing the conservation of the physical quantity that corresponds to the stock (e.g. nitrogen level).

- An output from an internal industrial process (e.g. digestate from anaerobic digestion), which may become input to another internal process or stock, can be estimated by an algebraic function of the input of the process, ignoring any internal accumulation within the industrial process.

- Exchange of resources and products with the external environment (e.g. import or chemical fertilizer), which is determined based on supply-demand balances.

Once the model equations are developed, implementation in a software tool is needed for running simulations. In a related work, stock-flow based modelling of local food-energy-water systems has been implemented in a spreadsheet based simulation tool called NexSym (Martinez-Hernandez, et al., 2017a). The present work adopted the MATLAB Simulink environment for model implementation and simulation of nutrient flows in a nexus system, in which the sophisticated mathematical models consisting of differential and algebraic equations can be solved efficiently.

3. Case study: building a model of nutrient flows and stocks for an eco-town in the UK

In this section, the conceptual characterisation and detailed models for an illustrative, simplified case study are presented, which makes use of the background information of an eco-town in the UK (Whithill and Bordon, 2012), in terms of the local demands, climatic conditions and resource (including land) availability. Figure 1 shows the overall conceptual structure of the nexus system analysed in this case study; these system components are assumed in this work, not based on the real situation as currently the actual local food and energy production is rather limited. Furthermore, the system is not intended to cover all the possible components but rather for providing a representative example. Also, nitrogen is the only representative nutrient chosen for analysis. The modelling approach can be readily extended to cover other nutrients such as phosphorous and potassium, in terms of the stock-flow structure and the general way of nutrient content accounting with different parts (e.g. straw and grain) of a crop and in different streams. However, the chemical transformation of these other nutrients during a whole nutrient cycle can be rather different, which needs to be addressed in an extended model.

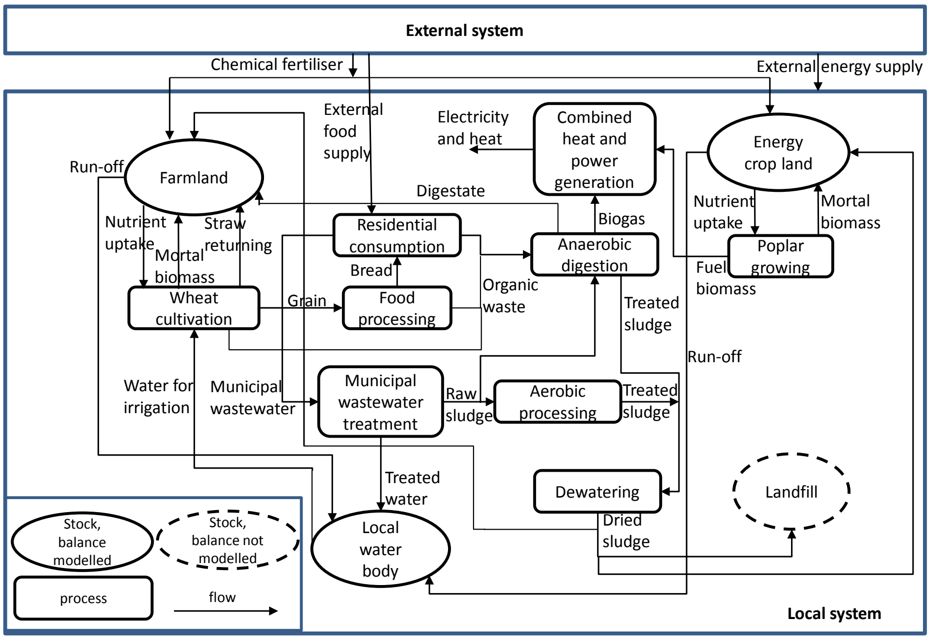


Figure 1. Conceptual structure for integrated food, energy and water production system.

The focus of the study is on analysing nutrient flows within the integrated local FEW system to assess the impact of various technical options and decisions on the consumption of nutrients-related resources and the associated environmental issues. In particular, the models were developed so that the integrated system can be simulated to assess the impact of the following factors:

a) Local food production – varying the local wheat supply level;

b) Local energy generation - introducing combined heat and power (CHP) + Anaerobic Digestion (AD), or CHP only; and

c) Nutrient recycle – varying the proportion of nutrient recycle by digestate application, and the proportion of wheat straw returned to soil.

The conceptual structures and mathematical modelling of individual nexus subsystems are described in detail in the following subsections.

3.1. Building conceptual structures

3.1.1. Conceptual structure of the food production subsystem

The conceptualised local food production system involves wheat cultivation on a farmland, with the harvested wheat being processed to white wheat flour as a source of carbohydrates for the local consumption. This food production system utilises the nutrients available from three different sources depending on the scenario analysed. The first source is the wheat straw used as an organic fertiliser after harvest, for the nutrients contained to be returned to the soil and utilised by the wheat plant. The second source is the digestate from an anaerobic digester introduced in the energy production system. The last resort, considered when the system is not completely self-sufficient in nutrient supply for the crop cultivation, is the use of chemical fertiliser. As there is no chemical fertiliser production unit designed in the local system, the use of it, if necessary, is based on importing from the external system.

3.1.2. Conceptual structure of the energy subsystem

The energy production subsystem includes a CHP plant to supply energy mainly to food cultivation, food processing, wastewater treatment, and the local residential sector. If there is an energy deficit in the subsystem, grid electricity from the external system is supplied to the internal system to fill the gap between the energy demand and the capacity of the local supply. On the other hand, excess energy, if any, could be exported to the external system. The CHP unit utilises biomass from energy crop cultivated locally and the biogas (with over 60% of methane) from a local anaerobic digester. Poplar has been chosen as the main energy crop based on its fast growth rate, high quality biomass (smaller proportion of bark) and modest requirement of fertilizer management (which nevertheless forms part of the nutrient demand quantified in this study).

3.1.3. Conceptual structure of water subsystem

The water subsystem in this case study is divided into two parts: a lake representing a local natural water body and the wastewater treatment processes. Water is supplied from the lake to food cultivation and processing, residential use and energy production, subject to the water quality regulation. Wastewater produced from different parts of the system is contaminated to various degrees and need to be treated before returning to the lake to avoid excessive accumulation of nutrients and toxic contaminants. In the water subsystem considered here, a simplified general-purpose wastewater treatment process is assumed to treat wastewater from residential, food and energy production processes together. The treatment train includes preliminary, primary, secondary and tertiary units. In recent years, an increasing attention has been drawn onto sludge treatment technologies. Sludge is generated during each single process of wastewater treatment and can be rich in nutrients. Given the limited space for direct disposal (landfill) of the sludge, sludge treatment and recycling of the embedded nutrients is considered.

3.1.4. Integrated structure of the food-energy-water nexus system

The food, energy and water subsystems conceptualised above have been connected by nutrient, water or energy flows, as shown in Figure 1. Even though not all possible system components are included in the structure, a rather intricate FEW system and nutrient linkages are captured. In particular, the energy and food subsystems are connected through the digester which is also fed by local food waste and organic waste from food processing (e.g. from wheat grain milling), and by agricultural residue from wheat cultivation if there is straw diverted from the return to soil. Such diversion could be either due to considerations in the appropriate fraction of the straw for return which may vary with agricultural practices and conditions (Liu, et al., 2013; Zhang et al., 2017), or as the consequence of deliberately increasing the application of the straw as feedstock for energy production (Townsend et al., 2017). The anaerobic digester is also used for sludge treatment in the wastewater treatment process. The multiple uses of the anaerobic digester lead to a large amount of digestate output which is rich in nutrients, and thus can be used to supply crops production and reduce the import of chemical fertiliser. There are also other important interactions between food and water subsystems, such as the use of nutrient sources originated from water treatment for the farmland, a fraction of which is subsequently transported into the water body through the runoff flows.

3.2. Mathematical modelling of the nexus subsystems

The next step of the case study is to quantify the processes and their interlinkages by mathematical models. The models are described for each of the nexus subsystems. The implementation and integration of the models are also discussed at the end of this section. It should be noted that the focus of the models developed in this work is primarily on mass balances of nutrients; important parameters such as yields or yield coefficients have been obtained from literature data as opposed to detailed modelling of relevant agricultural and industrial processes.

3.2.1. Modelling of the food subsystem

Nitrogen is one of the key elements to ensure the healthy growth of most plants and to increase crop yields. To satisfy the carbohydrates supply to the local residence through wheat cultivation, the stock of nitrogen in the soil needs to be monitored and kept in an appropriate level so that the growth potential of wheat is maximised and maintained. The balance of nitrogen stored in the soil, S_N (kg m^{-2}), is thus modelled as:

$$\frac{dS_N}{dt} = F_{Nin} + F_{Nmort} - F_{Nout} \tag{1}$$

where F_{Nin} (kg m^{-2}yr^{-1}) is the nitrogen flow into the soil;

F_{Nmort} is the mortality of wheat, which contributes to the nutrient accumulation in the soil;

F_{Nout} represents the removal of nutrient from the soil by growing the wheat.

F_{Nin} in Eq. 1 is the sum of nutrient inputs from all sources:

$$F_{Nin} = \left(F_{Nferti} + F_{Nsc} + F_{Nbio}\right)\left(1 - r_{runoff}\right) \tag{2}$$

where r_{runoff} indicates a certain fraction of nutrient running off the land to the local water body. A value of 0.2 has been adopted in the case study to represent an average level, although it may derivate from the actual levels of some specific cases as up to 80% of runoff of nitrogen from agricultural land has been observed (Howarth et al., 2002). F_{Nferti} (kg m^{-2} yr^{-1}) indicates the nitrogen brought in by the external chemical fertiliser, which is controlled based on the level of nitrogen stock in the soil. F_{Nsc} indicates a nitrogen enrichment by recycling the anaerobic digestate as a soil conditioner:

$$F_{Nsc} = F_{NinAD} * k_{SC} \tag{3}$$

where F_{NinAD} is the nitrogen contained in digestate after the anaerobic process, k_{SC} is the fraction of nitrogen left in the soil conditioner after conversion from the digestate.

F_{Nbio} indicates the nitrogen flow recycled through the straw returned to the soil:

$$F_{Nbio} = F_{Bout} * f_{Bstraw} * f_{Nstraw} \tag{4}$$

where F_{Bout} is the biomass harvested from the farmland, f_{Bstraw} is the fraction of straw out of the total biomass harvested, and f_{Nstraw} is the nitrogen content in the straw. F_{Bout} is modelled as:

$$F_{Bout} = F_{yield} * f_{harv} \quad (5)$$

where F_{yield} is the total standing biomass growing on the land, and f_{harv} represents the fraction to be harvested out of the total biomass.

F_{Nmort} in Eq. 1 is modelled as a function of the standing biomass and the nitrogen content:

$$F_{Nmort} = F_{yield} * r_{Bmort} * f_N \quad (6)$$

where r_{Bmort} is the fraction of the standing biomass that is littered. f_N represents the total nitrogen content in the wheat biomass, which is modelled as:

$$f_N = f_{Bstraw} * f_{Nstraw} + f_{Bgrain} * f_{Ngrain} \quad (7)$$

where f_{Bgrain} is the fraction of grain in the total biomass, and f_{Ngrain} is the nitrogen fraction in the grain.

F_{yield} (kgm^{-2}yr^{-1}) in Eq. 6 is modelled as a function of the nitrogen stock S_N in the soil:

$$F_{yield} = f(S_N) \quad (8a)$$

The relationship can be determined from known influence of soil nitrogen concentration on wheat grain yield, $F_{Grain\,Yield}$. In this work, a linear function is used according to literature data (Queensland Government, 2012):

$$F_{GrainYield} = k_{YC} * S_N \quad (8b)$$

where k_{YC} is a constant. The total standing biomass yield can then be obtained by a factor, f_{Bgrain}:

$$F_{yield} = F_{GrainYield}/f_{Bgrain} \quad (8c)$$

To finally complete the description of nitrogen balance in wheat-growing soil, F_{Nout} in Eq. 1 is modelled as:

$$F_{Nout} = F_{Bout} * f_N \quad (9)$$

Following cultivation, the wheat grain needs to be processed in the food production unit. The pericarps will be separated and supplied to the anaerobic digester, while wheat flour is supplied to human consumption. The nitrogen flow in the flour (F_{Nflour}) and the pericarp ($F_{Npericap}$) are modelled as:

$$F_{Nflour} = F_{Ngrain} * f_{Nflour} \quad (10)$$

$$F_{Npericap} = F_{Ngrain} * f_{Nperi} \quad (11)$$

where f_{Nflour} and f_{Nperi} are the fractions of nitrogen in flour and pericarp, respectively.

As mentioned earlier, chemical fertiliser is applied when local nutrient supply is not sufficient to meet the demand. In this work, a control system that represents nutrient management actions is implemented in Simulink to automatically determine the external chemical fertiliser application so that the nitrogen level in the soil can be kept in a desired level. In the case study, this level was set to be 0.036 kg/m^2, aiming to lead to a wheat grain yield of 7.906 tonnes/ha/yr, determined according to the literature yield data (Queensland Government, 2012). The parameters for the simulation of the food subsystem are summarised in Table 1.

Table 1. Parameters for the simulation of the food subsystem.

Symbol	Parameter	Value	Unit	Source
N_{target}	Target nitrogen concentration in wheat soil	0.036	kg m^{-2}	DEFRA, 2016
f_{Bgrain}	Fraction of grain out of the total biomass harvested	0.426		Guk and Kalkan, 2016
f_{Bstraw}	Fraction of straw out of the total biomass harvested	0.574		Guk and Kalkan, 2016
f_{harv}	Fraction of the total biomass harvested	0.95		Assumed
f_{Nstraw}	Nitrogen content in wheat straw	0.0104	kg kg^{-1}	Government of Alberta
f_{Ngrain}	Nitrogen content in wheat grain	0.0249	kg kg^{-1}	Government of Alberta
f_N	Total nitrogen contained in wheat	0.0166	kg kg^{-1}	Government of Alberta
f_{Nflour}	Fraction of nitrogen in flour	0.33		Conde Nast, 2014
f_{Nperi}	Fraction of nitrogen in grain pericarp	0.67		Conde Nast, 2014
k_{YC}	Yield coefficient of wheat grain	21.96	kg kg^{-1}	Queensland Government, 2012
k_{SC}	Fraction of nitrogen left in the soil conditioner	0.8		Assumed
r_{Bmort}	Fraction of the dead standing biomass	0.05		Assumed
r_{runoff}	Percentage runoff of nutrient	0.2		World Resources Institute, 2017

3.2.2. Modelling of the energy subsystem

Similar to wheat cultivation, nutrient stock of nitrogen in the soil for the energy crop poplar needs to be investigated as it affects the growth of poplar and consequently the amount of biomass feedstock for the CHP plant. Thus, the nitrogen stock is modelled in a similar way to Eq.1. In the case of poplar there is no straw returning to the land, thus the nitrogen input flow is modelled as:

$$F_{Nin} = (F_{Nferti} + F_{Nsc})(1 - r_{runoff}) \quad (12)$$

In this case, the F_{Nmort} term in Eq. 1 represents the mortality of poplar trees. It is assumed that the natural defoliation accounts as the mortality so the nitrogen introduced by this process comes mainly from poplar leaves:

$$F_{Nmort} = F_{Bout} * f_{Bleaf} * r_{Bmort} * f_{Nleaf} \quad (13)$$

where F_{Bout} is the total harvested poplar biomass, f_{Bleaf} is the proportion of leaves out of the total biomass, r_{Bmort} is the fraction of leaves that falls into the soil due to defoliation, and f_{Nleaf} represents the nitrogen fraction in poplar leaves.

F_{Nout} in this case represents the removal of nutrient from the soil by growing the poplars:

$$F_{Nout} = F_{Bout} * \left[f_{Bstem} * f_{Nstem} + f_{Bleaf} * (1 - r_{Bmort}) * f_{Nleaf}\right] \quad (14)$$

where f_{Bstem} is the proportion of stem biomass out of the total biomass, and f_{Nstem} represents the nitrogen concentration in poplar stems.

As in the case of wheat, F_{Bout} (kg m^{-2} yr^{-1}) is modelled as a function of the nitrogen stock S_N in the soil. However, the relationship is much more complicated in the case of poplar. Firstly, the diameter at breast height (DBH, in cm) is related to the nitrogen concentration in soil, by a linear regression model based on the experimental results reported in Fang et al. (2008):

$$DBH = 148.6 S_N \frac{d}{\rho} + 10.11 \quad (15)$$

where the soil depth (d, in m) and soil density (ρ, in kg/m^3) are introduced to covert the nitrogen content per unit area of soil (i.e. S_N, in kg/m^2) to per unit mass of soil (kg/kg). Subsequently, the DBH is related to the dry weight per tree (in kg), by a linear regression model based on the experimental results reported in Byrd (2013):

$$Dry\ weight = 0.116 DBH - 0.0744 \quad (16)$$

After this, multiplying the dry weight per tree by the number of poplar trees planted per m^2 and percentage of lumbering per year, the dry mass produced per year can be found. A conversion between dry mass to fresh mass is needed because the data used for nutrient content and fractions of stems and leaves were obtained on a wet mass basis. As in the food subsystem, a control system is implemented so that chemical fertiliser import and application can be controlled to maintain the nitrogen content in the soil to a pre-specified level. In the case study, this level was set to be 0.624 kg/m^2, aiming to lead to a poplar biomass yield of 4.241 tonnes/ha/yr, determined according to the literature yield data (Fang et al., 2008; Byrd, 2013).

The lumbered poplar trees are delivered to the combined heat and power (CHP) plant. In the CHP component, most of the nitrogen element ends up in the atmosphere in several possible forms such as N_2, NH_3, and NOx (Salzmann and Nussbaumer, 2001), with the remaining fraction assumed to become part of the ash. Note that the accumulation of nitrogen-containing species in the atmosphere is not modelled in this work. The parameters for the simulation of the energy subsystem are summarised in Table 2.

Table 2. Parameters for the simulation of the energy subsystem.

Symbol	Parameter	Value	Unit	Source
N_{target}	Target nitrogen concentration in poplar soil	0.624	kg m^{-2}	Morhart et al., 2013
f_{Bleaf}	Fraction of leaves out of the total energy crop harvested	0.0952		Poorter et al., 2011
f_{Bstem}	Fraction of stems out of the total biomass harvested	0.9048		Poorter et al., 2011
f_{Nleaf}	Nitrogen content in poplar leaves	0.0072	kg kg^{-1}	Salehi et al., 2013
f_{Nstem}	Nitrogen content in poplar stem	0.00302	kg kg^{-1}	Morhart et al., 2013
r_{Bmort}	Fraction of deciduous leaves	0.2		Assumed
ρ	Soil density	1600	kg m^{-3}	Hunt and Gilkes, 1992
d	Soil depth	0.2	m	Morhart, et al., 2013
n	Number of trees per acre	1500		Law et al., 2012
f_{lumb}	Fraction to be lumbered	0.5	$year^{-1}$ (coppiced)	Assumed
r_{runoff}	Percentage runoff of nutrient	0.05		Dong et al., 2014
K_{fd}	Conversion from fresh to dry biomass	2		eXtension, 2014
$f_{CHPout1}$	Fraction of CHP nitrogen outlet to air	0.8		Assumed
$f_{CHPout2}$	Fraction of CHP nitrogen outlet to ash	0.2		Assumed

3.2.3. Modelling of the water subsystem

In the wastewater treatment process, the nitrogen contained in the inlet wastewater flows is distributed into various output flows. This is modelled as:

$$N_{raw\ in} = N_{sludge} + N_{air} + N_{tw} \quad (17)$$

$N_{raw\ in}$ is the nitrogen contained in the raw influent combining wastewater from residential, food processing and energy production components, and is determined by the product of the volume of the raw wastewater (V_w) and its nitrogen content (C_{Nraw}):

$$N_{raw\ in} = V_w * C_{Nraw} \quad (18)$$

N_{sludge} is the nitrogen that ends up in the sludge. N_{air} is the nitrogen released to the atmosphere, primarily in the form of N_2. N_{tw} represents the nitrogen left in the treated water and must meet the regulatory standard. Each output can be calculated by a fraction factor of $N_{raw\ in}$, such as f_{sludge} (the fraction entering sludge), f_{air} (the fraction entering air) and f_{tw} (the fraction entering treated water).

Sludge resulting from wastewater treatment is further treated. The nitrogen content in a treated sludge stream depends on the sludge treatment method adopted, which is indicated by the fraction f_{treat}:

$$N_{treated\ s} = f_{treat} * N_{sludge} \quad (19)$$

where $N_{treated\,s}$ is the nitrogen content in the treated sludge. Considering anaerobic and aerobic sludge treatment as two different options, f_{treat} can be obtained by

$$f_{treat} = (f_{ant} \; or \; f_{at}) * f_{de} \tag{20}$$

where f_{ant} and f_{at} are proportions of nitrogen remaining in anaerobically and aerobically treated sludge, respectively; f_{de} is the remaining fraction of nitrogen following a subsequent dewatering step. Sludge from wastewater can also be composted to obtain biosolids for agricultural uses, although this option is not modelled here. In some scenarios studied in this work, at least some of the sludge is sent to landfill which is simply taken as a sink of this stream; its environmental impact is not modelled.

The treated wastewater is discharged to the lake, so the nutrient transformation and accumulation in this local water body needs to be modelled. The process simulated in the lake is simplified to the aggregated removal of nutrients quantified through the apparent settling velocity (Neitsch et al., 2005). The total balance of nutrient concentration in the water body, c, can then be expressed as:

$$\frac{dc}{dt} = \frac{1}{V}[W - Qc - vcA_s + r] \tag{21}$$

where V (m^3) is the water body volume, assumed to be constant, W(kg yr^{-1}) is nutrient entering the water body, Q ($m^3 yr^{-1}$) indicates the water exit flow which can be due to withdrawal to cover local water demand, r (kg yr^{-1}) shows the annual nutrient runoff from the food and energy crop land. The modelling of the loss of nutrient by settling involves v (m yr^{-1}) as the settling velocity of the nutrient, and A_s as the area of sediment-water interface.

The parameters for the simulation of the water subsystem are summarised in Table 3.

Table 3. Parameters for the simulation of the water sub-system.

Symbol	Parameter	Value	Unit	Source
V_w	Wastewater volume	1,110,158	$m^3\ yr^{-1}$	Leung Pah Hang et al., 2016
C_{Nraw}	Nitrogen concentration in raw wastewater	0.0135	$kg\ m^{-3}$	Assumed
f_{sludge}	Proportion of nitrogen end up in sludge	0.3333		Bloch, 2001; Grant, 2014
f_{air}	Proportion of nitrogen end up in air	0.4666		Law et al., 2012
f_{tw}	Proportion of nitrogen left in treated wastewater	0.2		Bloch, 2001; Grant, 2014
f_{ant}	Proportion of nitrogen left in anaerobic treated sludge	0.3		EPA, 1996
f_{at}	Proportion of nitrogen left in aerobic treated sludge	0.1		EPA, 1996
f_{de}	Proportion of nitrogen left after dewatering	0.2		EPA, 1996
V_w	Volume of treated water to discharge	1.110e6	$m^3\ yr^{-1}$	Assumed
Q	Volume of water withdrawal	2.605e6	$m^3\ yr^{-1}$	Specified
f_q	Proportion of water supply from the lake	0.64		Leung Pah Hang et al., 2016
v	Nutrient settling rate	20	$m\ yr^{-1}$	Neitsch, 2005
V	Volume of lake system	314.3e6	m^3	Guide, 2017
A_s	Area of sediment-water interface	14.7e3	m^2	Guide, 2017

3.2.4. Model implementation, integration and the case study settings

The mathematical models and their parameterisation for individual subsystems were first implemented separately in MATLAB Simulink. Thereafter, model integration was carried out to allow the simultaneous simulation of the interconnected nexus system. MATLAB Simulink enables direct and convenient linkage between the different systems. In this particular case, three additional actions were required for the model integration to represent the overall structure of the integrated system (Figure 1). Firstly, the surface runoff from both farmland and energy crop lands needed to be combined as nutrient input to the local lake. Secondly, the anaerobic digesters used in both the food waste processing and wastewater treatment could now be combined into a single unit, but with multiple inputs. Thirdly, data for the specific locale being investigated needed to be incorporated into the model, such as population and land availability.

In the case study, a period of 50 years has been simulated. The initial levels of nitrogen in the lands for growing wheat and poplar, as well as the initial nitrogen concentration in the local lake, are given in Table 4. Throughout the simulated period and across different levels of local food production simulated, the total amount of locally generated wastewater and its nitrogen content (hence potential for nutrient recovery) was kept constant (as given in Table 3), with the assumption that the variations between these different scenarios would have a minimum impact on the total discharge of nitrogen into the municipal wastewater system.

Table 4. Initial conditions adopted in the simulation.

State	Initial value
Nitrogen level in land for growing wheat	0.0137 kg/m^2
Nitrogen level in land for growing poplar	0.1952 kg/m^2
Nitrogen concentration in lake	0.25e-3 kg/m^3

The specificities of population, land available, energy, flour and water demand of the case study locale are given in Table 5.

Table 5. Local specificities adopted in the simulation.

Specificities	Value
Population	17,000
Land available for food and energy crop	87 ha, with 17 ha occupied for food crops in the existing system
Residential electricity demand	9.0e5 GJ yr^{-1}
Average total wheat flour demand (for bread making)	284.5 t yr^{-1}
Total water demand	2.6e6 t yr^{-1}
Wastewater discharge required at < 0.1 g COD/kg	1.1e6 t yr^{-1}

4. Results and discussion

The models were solved to simulate the individual subsystems first. Subsequently, several scenarios were analysed through simulations of the integrated FEW system.

4.1. Simulation of individual subsystems

The subsystems were simulated without nutrient recycle flows across the subsystems but with recycle within subsystems. In the food subsystem the nitrogen flows are: imported chemical fertiliser, wheat straw returned to soil in farmland, nutrient in food waste going to anaerobic digestion (AD), and the digestate from AD used as fertiliser to wheat cultivation. Note that in this case a separate digester for food waste is considered as part of the food production subsystem only. The stock of interest in the food subsystem is the nitrogen content in the soil for growing wheat. As shown in Figure 2(a), this nitrogen stock evolves in 10 years or so from its initial level (0.0137 kg/m^2) to a stable level (0.036kg/m^2), driven by various nitrogen inputs to soil. This steady state value determines the annual wheat (grain) yield and straw return rate of 7.91 and 10.13 tonnes/ha/yr, respectively. With 17 ha of agricultural land available in the locality, the local wheat production can only supply 15% of the total demand.

The main nutrient flows in the food subsystem are also stabilised at the steady state, with the individual flows from the food waste anaerobic digestate, straw and chemical fertiliser being 1.5×10^{-2}, 1.05×10^{-2} and 9.14×10^{-3} $kg/m^2/yr$, respectively. Note that most of the fertiliser required is provided by the local sources (74%), while imported chemical fertiliser contribution is 26%. It is clear that, by recycling food waste anaerobic digestate and straw alone, significant reduction in imported chemical fertiliser can already be achieved. A complete substitution of imported fertiliser will require recycling from other local resources, such as digestate from AD of wastewater treatment sludge, which will be discussed later.

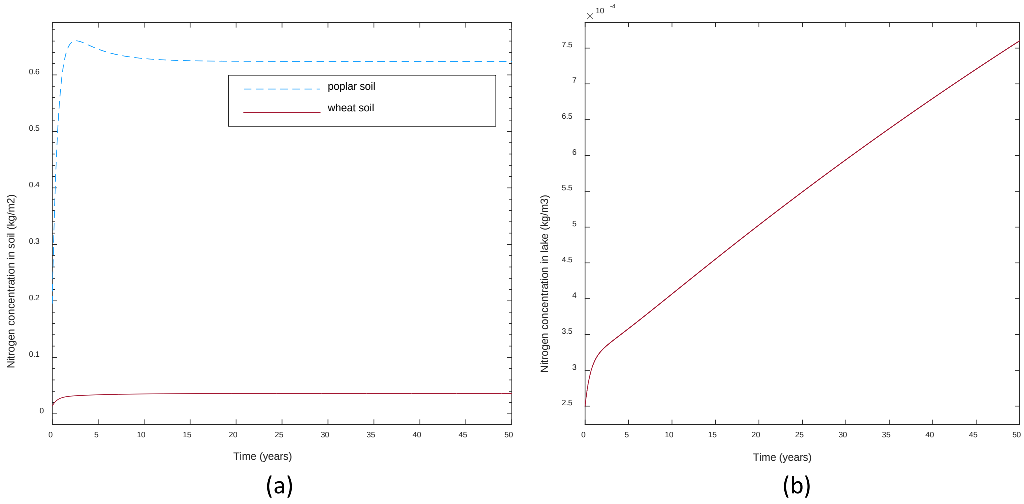


Figure 2. Evolvement of nutrient stocks. (a) Nitrogen stock in soils; (b) nitrogen stock in the lake.

In the energy production subsystem, the nitrogen stock of interest is that in the soil for growing poplar. As shown in Figure 2(a), it also takes about 10 years to evolve from its initial level (0.195 kg/m^2) to a stable level (0.624 kg/m^2). At the steady state, poplar appears to require chemical fertiliser at only 1.46×10^{-3} $kg/m^2/yr$, which is significantly lower compared to the previously mentioned value for wheat cultivation (9.14×10^{-3} $kg/m^2/yr$). The lower application of chemical fertiliser, together with a better retention ratio, leads to a lower runoff value for the poplar cultivation land reaching 7.56×10^{-5} $kg/m^2/yr$ at the steady state, compared to the runoff value from wheat cultivation at 6.93×10^{-3} $kg/m^2/yr$. Therefore, less pollution to the water body is expected from poplar cultivation in the energy subsystem.

In the water subsystem, the two main components are the lake as the local water body and the wastewater treatment processes, including sludge treatment. The simulation reveals that at the steady state, the level of nitrogen concentration in the treated water stabilises at the value of 2.73 $\times10^{-3}$ kg/m^3, which satisfies the EU regulation (Bloch, 2001). Nevertheless, the discharge of this treated water stream to the local lake causes a continuous increase in the nitrogen concentration (or stock) in the local water body from 2.54×10^{-4} to 7.53×10^{-4} kg/m^3 in the period of 50 years, a significant increase of 200%, as shown in Figure 2(b). The excess nitrogen input into the lake could cause overstimulation of the growth of aquatic plants and algae. The excessive growth of these organisms, in turn, can clog water intakes, use up dissolved oxygen as they decompose, and block light to deeper waters, ultimately leading to eutrophication. Thus, it is important to look at the whole FEW system in an integrated approach to identify critical flows and processes from the food and energy subsystem that affect the stock of nutrients in the ecological components of the water subsystem. Once this information is obtained, techno-ecological interventions to minimise or balance any excess or deficits of nutrients in the systems can be devised. This type of integrated assessment is explored in various scenarios in the next section.

4.2. Scenario analysis using the integrated nexus model

The integrated model of the food-energy-water nexus allows performing simulations for a holistic analysis of the local system. In this case study, the integrated analysis has been focused on scenarios defined along three different factors to investigate the variations in nitrogen stocks and flows and their resource and environmental implications. The three dimensions are: a) level of local food supply; b) selection of energy generation technologies, and c) level of nutrient recycle through digestate and straw. Table 5 shows the ranges of values or options used for scenario analyses and the values used in the base case scenario. It should also be noted that, each scenario (investigated in section 4.2.2, 4.2.3 or 4.2.4) adopts all the base case parameter values, except for the parameter that the scenario is particularly focused on. Given that the system is able to reach steady state around year 10 (except the local lake), the values at year 50 are taken to predict the nutrient flows at the steady state. Unless stated otherwise, the magnitudes of nutrient flows presented in Section 4.2 are all steady-state figures.

Table 5. Factors investigated in the scenario analysis.

<table>
<tr><th>Factor</th><th>Range of Analysis</th><th>Base-case value</th></tr>
<tr><td>Local food (wheat) supply level (proportion of total demand)</td><td>0% - 44%</td><td>44% (using 50 ha of land)</td></tr>
<tr><td rowspan="2">Energy generation technologies</td><td>1) Combined heat and power (CHP) + Anaerobic digestion (AD)</td><td rowspan="2">CHP + AD</td></tr>
<tr><td>2) Combined heat and power (CHP) only</td></tr>
<tr><td rowspan="4">Nutrient recycle</td><td colspan="2">Anaerobic digestate</td></tr>
<tr><td>0% - 100%</td><td>100%</td></tr>
<tr><td colspan="2">Straw returning</td></tr>
<tr><td>0% - 100%</td><td>100%</td></tr>
</table>

4.2.1. Base case

The base case scenario considers using up to 50 ha (out of 87 ha available for food and energy crops) for wheat cultivation, which allows supplying the maximum of 44% of local wheat flour demand. This leaves only 37 ha of land for poplar cultivation. The base case scenario also considers the use of AD+CHP plant for nutrient recovery and energy generation, and the use of 100% digestate and straw returning to soil. Figure 3 shows the resulting nutrient input and outputs of the integrated nexus system (without showing the flows recycled internally) at the steady state (i.e. at year 50).

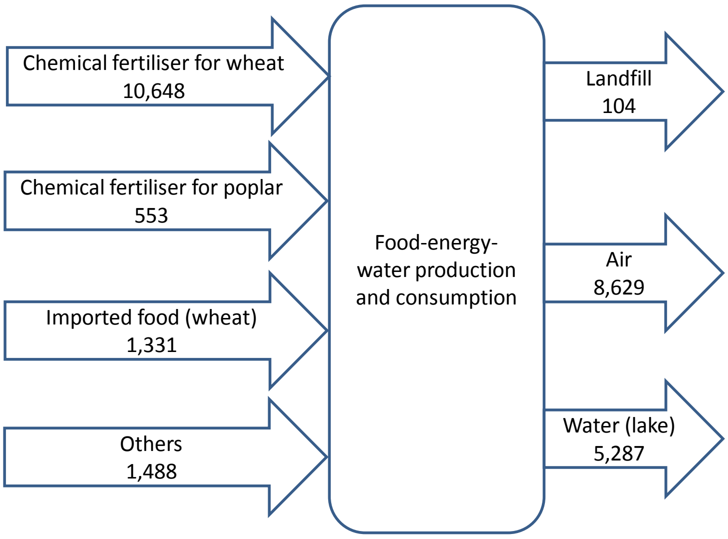


Figure 3. Nitrogen inlet and outlet flows in the nexus system, base-case scenario (unit: kg nitrogen/year).

The significant amount of the imported chemical fertiliser indicates that recycling of nitrogen within the system is not enough to cover all the nitrogen needs for wheat and poplar cultivation. The 'Others' stream represents other external nutrient sources than those explicitly considered in the model, such as imported foods other than wheat, which would contribute to the nitrogen content of the municipal wastewater. On the output side, most of the "lost" nitrogen ends up in air and the local water body; only a small amount goes to landfill, thanks to the internal circular use of nitrogen captured from waste and residual streams.

4.2.2. Effect of local food production

As observed in the results from the simulation of the individual subsystems, the main effect of local wheat cultivation is on the flows of chemical fertiliser needed and the flows recycled through digestate and straws. As expected, the higher the local food supply, the higher the need for fertilisers and the straw available for returning to land, as shown in Figure 4. One effect of producing less local wheat is that more land becomes available for poplar cultivation used in energy production. As poplar cultivation is less demanding in chemical fertiliser than wheat cultivation, this would lead to less import and application of chemical fertilisers. This in turn will affect the nitrogen flow in runoff and the resulting concentration in the lake, as shown in Figure 5. For example, if local wheat production is at 44% (base case), the nitrogen concentration in the lake at year 50 will be nearly 70% higher than the case with no local wheat production. On the other hand, as more poplar is produced using the land available, more nitrogen will be emitted through combustion in the CHP plant, leading to about 5% increase in nitrogen flow to air. Overall, an increased level of local wheat production is most likely to be accompanied by a higher total nitrogen rejection to the local environment due to the runoff from land, as long as the application of chemical fertilisers is indispensable. In such cases, it is critical to implement runoff management strategies so that the potential nutrient pollution to the local water body can be avoided. Such local considerations, however, need to be balanced with the external impact of certain decisions. For example, a reduced level of local production may ease local pollution, however at a cost of increased pollution in exporting regions.

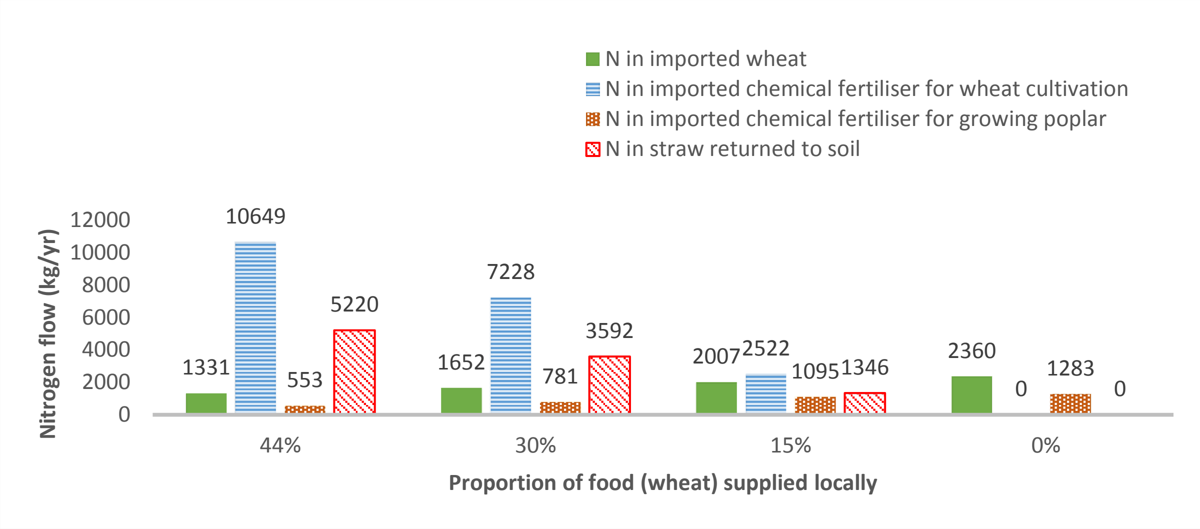


Figure 4. Impact of the proportion of local food supply on nitrogen flows.

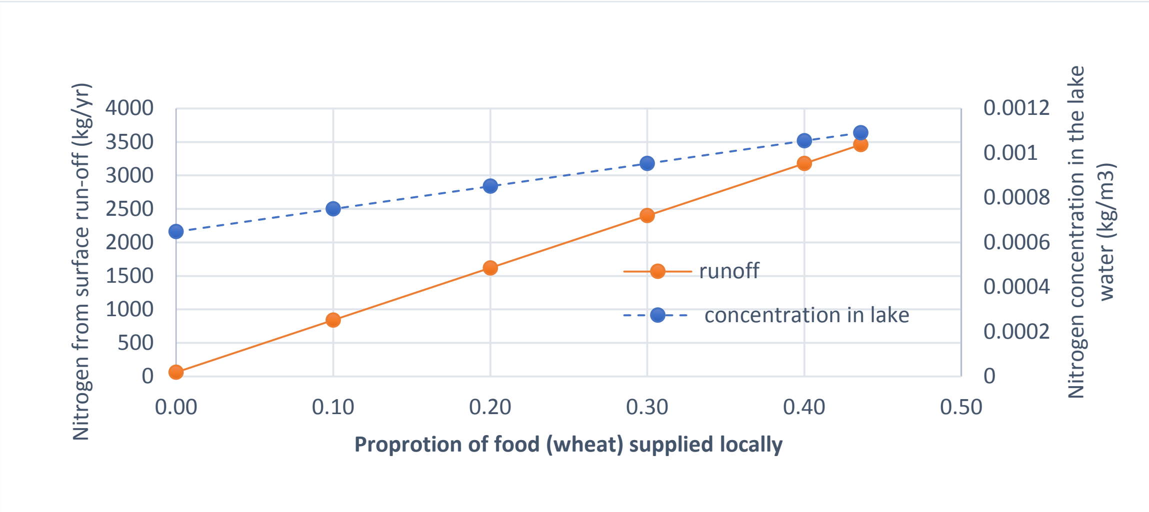


Figure 5. Nitrogen in runoff and nitrogen concentration in local lake at varying proportions of food (wheat) supplied locally.

4.2.3. Effects of the selection of energy generation technologies

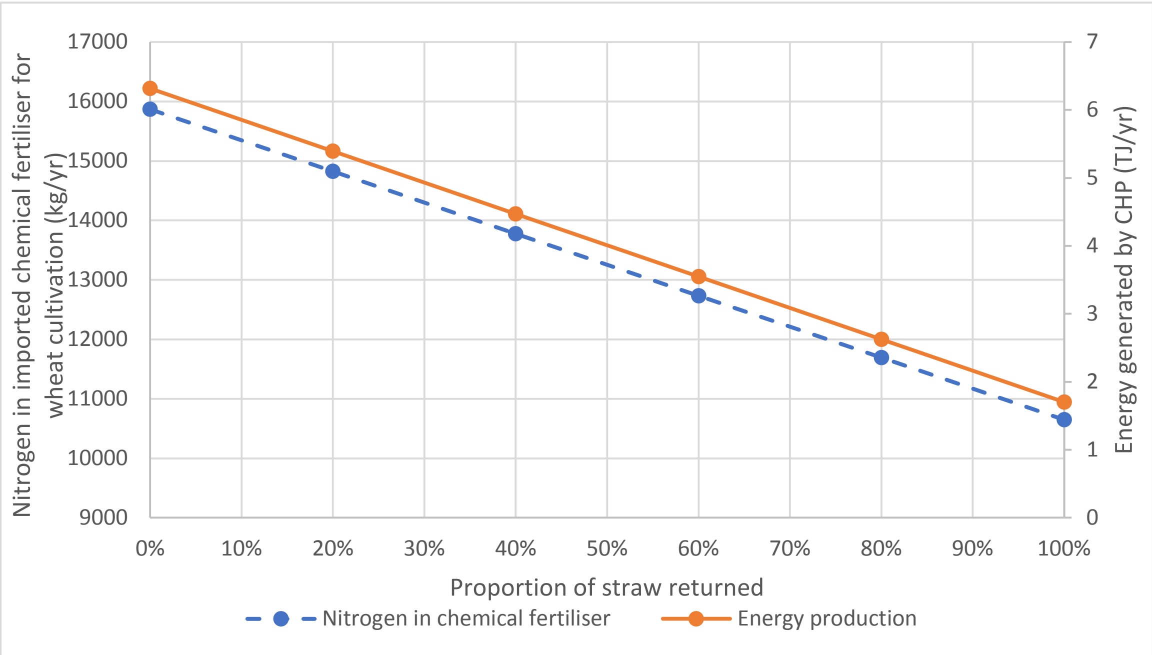
In this part of the analysis, the main objective is to achieve a quantitative understanding of the benefit brought by introducing an AD unit. Thus, the two options explored are (i) a CHP plant with an AD unit (as in the base case scenario) and (ii) CHP without AD. It is evident that the inclusion of AD into the system helps to boost energy production. Moreover, the use of AD in food waste processing and sludge treatment is nutrient-beneficial as the anaerobic digestate can be recycled to the farmland. At the steady state (i.e. at year 50), the energy generated by combusting poplar is around 1.46 TJ every year. Combustion of the biogas generated by the case including an AD unit could additionally provide 0.24 TJ energy to the locale.

Without the returning of the nutrient-rich anaerobic digestate, the simulation shows about 10% increase in the chemical fertiliser nitrogen demand for wheat cultivation, compared to the base case scenario. The system without the AD unit has further impact on the nitrogen output: The landfill nitrogen increases dramatically from 104 (with AD) to 6,315 kg/yr (without AD).

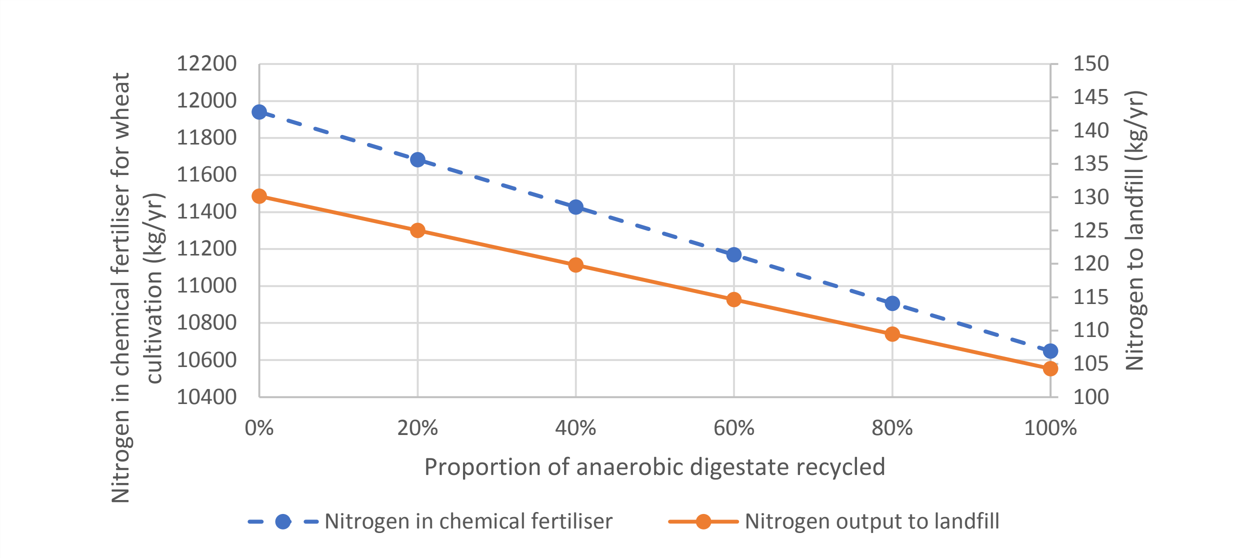
To summarise, the CHP + AD combined technology can help to generate more energy given the same resources, reduce the chemical fertiliser importation to the system, and reduce the amount of nitrogen entering landfilled.

4.2.4. Effect of nutrient recycle level

The main resources of nutrient recycle in the system are the anaerobic digestate recycled following sludge treatment and food waste treatment, and the straw returned to the agricultural land. In this subsection, the impact of different degrees of nitrogen recycling within the integrated system is analysed. Results in Figure 6(a) show that straw can be a major source of nutrient recycle, capable of reducing imported fertiliser by up to one third compared to the non-recycle case. Unlike AD, straw returning does not involve a complex treatment process. On the other hand, even though straw returning is of benefit in terms of nutrient, a trade-off should be made with other potential uses, in particular energy generation. Wheat straw is a raw material that can be used in the CHP unit for energy generation. Figure 6(a) also shows that a full use of straw in the CHP (0% recycle to the land) can generate 4.61 TJ of energy per year (corresponding to the difference in energy generation between 0% and 100% straw returning). This represents a significant power generation capacity. Therefore, a decision on the proportion of straw recycled to the land should be made with considerations of factors such as total energy demand, cost of recycle, and cost of external electricity and fertiliser. Besides, the simulation also showed that returning a lower proportion of straw to soil with a diversion to CHP would generate more nitrogen losses to the air due to burning and more losses to landfill via the disposal of ashes, hence an increased environmental impact. It should be noted that this analysis has only considered the role of returning straw to land in nutrient recycle; its wider impact on soil health (e.g. Liu et al., 2013) has not been included. Regarding the anaerobic digestate, Figure 6(b) shows that 100% recycle can reduce the chemical fertiliser consumption by 10.8% compared to non-recycle while reducing sludge going to landfill, leading to about 20% reduction of landfilled nitrogen.



(a)



(b)

Figure 6. Impact of the level of nutrient recycle. (a) Nitrogen in chemical fertiliser for wheat and energy production varying with the proportion of returned straw; (b) nitrogen input by chemical fertiliser for wheat, and nitrogen output to landfill varying with the proportion of recycled anaerobic digestate.

5. Conclusions

In this paper, nutrient flows and stocks in a local food-energy-water system have been modelled. Starting from generating conceptual structures, mathematical models of sub-systems and the overall integrated system were developed. The integrated nexus system model was used to conduct simulations of an exemplary local FEW system under several scenarios differentiated in the level of local food supply, selection of energy technologies, and the level of recycling of straw and digestate. The analysis of varying the proportion of food produced locally revealed its significant impacts on the nitrogen chemical fertiliser import, the surface nutrient runoff, and the nitrogen stock in the local water body. From the simulation of different options for energy production, it was clear that the adoption of anaerobic digestion would not only help to generate more electricity but also greatly reduce the nutrient imported and landfilled. In the analysis of nutrient recycle by varying the percentages of straw returning and anaerobic digestate, it was shown that the anaerobic digestate should be recycled to minimise the landfill burden, while a balanced decision needs to be made on the straw returning rate considering its implications on energy generation potential and fertiliser importing.

More generally, the results obtained in this study demonstrated the role of nutrient flows and stocks in interlinking the food, energy and water subsystems and the importance on tracking their dynamics to prevent impacts on the surrounding environment. However, it needs to be noted that this work has focused on the technical perspective; other factors such as the economic cost and social impacts will need to be taken into consideration in order to comprehensively inform sustainable decisions.

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