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# Sustainable energy-water-food nexus integration and optimisation in eco-industrial parks

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ABSTRACT

In this study, a representation of the Energy-Water-Food (EWF) nexus is developed to capture the trade-offs and synergies between sustainability dimensions within an industrial park. A unique systems approach based on thermodynamics is developed to optimise the nexus and enhance resource efficiency. The case study involves various chemical processes operating in the State of Qatar, which is evaluated to ascertain resource efficiency enhancement possibilities across various scenarios, and considers multiple objectives to capture the trade-offs between minimising the total annual cost and environmental emissions. Furthermore, a sustainability metric is applied to compute the effect of each scenario on EWF resources. In this study, there is emphasis on capturing the synergetic potential from utilising biomass from the food sector. The results indicate that the global warming potential in the best performing scenario decreases by approximately 30 %, while the exergy efficiency of the system is enhanced by 28 %.



## 1. Introduction

As the global population is expected to increase to 9 billion by 2050, it is expected that agricultural activities will need to expand by 70% to satisfy the demand of the population (Karan et al., 2018), whilst water and energy footprints rise in parallel. Today, food production systems account for 70 % of total global freshwater withdrawals and 30% of the total energy consumed globally (Mancosu et al., 2015). Incidentally, the global energy production in 2010 accounted for 15% of global freshwater withdrawals. Evidently, there are interdependencies and trade-offs that exist across Energy-Water-Food (EWF) sectors in what is known as the 'nexus' of the three resources, which was first introduced at the Bonn Nexus Conference in 2011 (Dombrowsky, 2011). For instance, energy is required to produce and distribute fresh water. Within the food sector, the demand for both water and energy resources are necessary for irrigation, production of fertilisers and to operate farms and machinery.

In an industrialised world, natural resources are utilised across various systems to produce value added products and services. In a linear system, natural resources are depleted and wastes are not utilised, which results in an inefficient and environmentally costly system. Globally, more than 1.9 billion metric tonnes of solid waste is produced annually (Atlas, 2018), which leads to major environmental impacts and economic costs (Manfredi and Cristobal, 2016). In support of sustainable development; industrial ecology and eco-industrial parks can guide towards more sustainable industrialisation. They promote cooperation between multiple number of plants by resource exchange, waste integration and the utilisation of sustainable resources with the objective of transforming the structure and operation of industrial parks from traditional linear (open loop) systems to closed/circular systems (closed loop), where wastes are decreased and reused as inputs for other processes (Lowe and Evans, 1995).

Biomass is a typical by-product from various urban and industrial processes, the recycling of which can reduce the carbon emissions associated with fossil fuels by approximately 20% (Daioglou et al., 2014). Biomass can be converted into useful biofuels and chemicals within various biorefinery processes that operate on the basis of industrial ecology principles. In such biorefinery processes, the waste is integrated and converted to powers, fuels, and chemicals. An integrated waste biorefinery that operates on the basis of industrial ecology principles can contribute towards the development of eco-industrial parks and circular economies. Benefits are obtained through land saving, energy generation, GHG

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**Nomenclature**

*Indices*

| | |
|---|---|
| $p$ | Plant/Process |
| $i$ | Water Source |
| $j$ | Water Sink |
| $s$ | Centralized Treatment |
| $l$ | Freshwater Type |
| $t$ | Central Treatment Type |
| $c$ | Contaminant |

*Sets*

| | |
|---|---|
| P | ($p$=1, 2, 3, …, S is a set of plants/processes) |
| I | ($i$=1, 2, 3, …, S is a set of water sources) |
| J | ($j$=1, 2, 3, …, S is a set of water sinks) |
| H | ($h$=1, 2, 3, …, S is a set of energy sources) |
| O | ($o$=1, 2, 3, …, S is a set of energy sinks) |

*Parameters*

| | |
|---|---|
| $z^{min}_{cj,p}$ | Minimum permissible pollutant c composition in sink j, plant p (ppm) |
| $z^{max}_{c,jp}$ | Maximum permissible pollutant c composition in sink j, plant p (ppm) |
| $G_{jp}$ | Flowrate required in sink j, plant p (kg/h) |
| $W_{ip}$ | Flowrate available in source i, plant p (kg/h) |
| $x^{Source}_{c,ip}$ | Pollutant c composition in source i, plant p (ppm) |
| $x^{FRESH}_{c,l}$ | Pollutant c composition in External Freshwater of type $l$ (ppm) |
| $R_{st}$ | Water recovery factor in centralized treatment s, type t |
| $RR$ | Removal Ratio |
| $x^{WW\_Max}_{c}$ | Maximum permissible discharge concentration of pollutant c in wastewater discharge |
| $x^{B\_Max}_{c}$ | Maximum permissible discharge concentration of pollutant c in brine discharge |

*Variables*

| | |
|---|---|
| E | Energy |
| $z^{in}_{c,jp}$ | Pollutant c Composition in sink j, plant p (ppm) |
| $M_{ip,jp'}$ | Water flowrate from source i, plant p to sink j plant p'(kg/h) |
| $F_{l,jp}$ | External freshwater flowrate of type l required in sink j, plant p (kg/h) |
| $D_{ip}$ | Wastewater flowrate discharged by source i, plant p (kg/h) |
| $T^{Inlet}_{ip,st}$ | Water flowrate from source i, plant p into central treatment s of type t (kg/h) |
| $T^{Treated}_{st,jp}$ | Treated water flowrate produced by central treatment s of type t sent to sink j, plant p (kg/h) |
| $D^{Treated}_{st}$ | Treated water flowrate sent to waste by central treatment s, of type t (kg/h) |
| $D^{Untreated}_{st}$ | Untreated (brine) water flowrate sent to brine waste by central treatment of type t (kg/h) |
| $WW^{total}$ | Total Wastewater Discharge (kg/h) |
| $B^{total}$ | Total Brine Discharge (kg/h) |
| $x^{Treated}_{c,st}$ | Concentration of contaminant c in the treated water stream produced by centralized treatment s, of type t (ppm) |
| $x^{Treated}_{c,st}$ | Concentration of contaminant c in permeate stream produced by central treatment s, type t (ppm) |
| $x^{Untreated}_{c,st}$ | Concentration of contaminant c in brine stream produced by central treatment s, type t (ppm) |
| $x^{WW\_Discharge}_{c}$ | Total wastewater discharge concentration of contaminant c |
| $x^{B\_Discharge}_{c}$ | Total brine discharge concentration of contaminant c |

emissions reduction, and resources management (Nizami et al., 2017). There are different technologies that can process and recycle biomass into the sustainable products, such as pyrolysis and gasification, which are well established processes for the production of syngas, oils and biochar. Syngas is produced from the gasification process, which can be used for power generation or production of clean fuels. It can substitute natural gas in combustion processes, gas to liquid (GTL), ammonia, and methanol processes (AlNouss et al., 2020). Notably, biomass waste produced from within the food sector, i.e. manure and food waste can be used as a feedstock for the gasification process. Biochar, a product from the biomass recycling process, is produced from either the pyrolysis or as a by-product form the gasification process (Pradhan et al., 2020). Biochar is a solid material that has the potential to improve the condition of soils for agriculture purposes by enhancing the water retention capacity (Lehmann and Joseph, 2009). The pyrolysis process has higher biochar yields and lower environmental emissions than the gasification process (Pradhan et al., 2020). However, the quality of obtained biochar depends on the process condition and feedstock (Elkhalifa et al., 2019). Fig. 1 illustrates the feedstock and products for both technologies.

## 2. The EWF nexus

The development of models that represent the EWF nexus can contribute towards effective resource management, balance trade-offs between resources and reduce environmental burdens from resource utilisation. In the recent years, the EWF nexus has been explored through various avenues, categorised into: life cycle assessment (LCA) studies (Mannan et al., 2018; Salmoral and Yan, 2018; Al-Ansari et al., 2015; Yuan et al., 2018), decision making tools (Namany et al., 2019; Bieber et al., 2018), multi scale studies (Garcia and You, 2016), and optimisation of the nexus (Al-Obaidli et al., 2019; Al-Thani et al., 2020; Lahlou et al., 2020), noting that most analysis within EWF nexus studies have focused on resource efficiency and environmental emissions (De Laurentiis et al., 2016). Within the energy-water nexus, Al-Obaidli et al. (Al-Obaidli et al., 2019) evaluated multiple desalination and power configurations considering fossil fuels and renewable energy sources to obtain an optimal configuration which decreases $CO_2$ emissions and costs. The results demonstrate that current configurations are suboptimal, and that the integration of renewable energy sources into the combined power and desalting plant (CPDP) infrastructure significantly improves $CO_2$ emissions, with improvement ranges between 52% and 67%, whilst the overall system levelised cost decreases between 8% and 32%. Various studies have considered the utilisation of biomass from the energy-food nexus perspective. For instance, AlNouss et al. (AlNouss et al., 2020; AlNouss et al., 2020) developed and optimised a syngas generating biomass gasification process using an Aspen Plus simulation model. Within this study, various biomass feedstock and operating conditions were considered. A sensitivity analysis was implemented to analyse the effect of operating conditions on the biomass gasification process. Moreover, AlNouss et al (AlNouss et al., 2020; AlNouss et al., 2019) compared two different gasification technologies (stream and oxygen) for biomass utilisation through techno-economic-environmental study for a poly-generation system. The poly-generation system uses biomass feedstock of different sources in order to generate electricity, Fisher-Tropsch liquids, and prod-

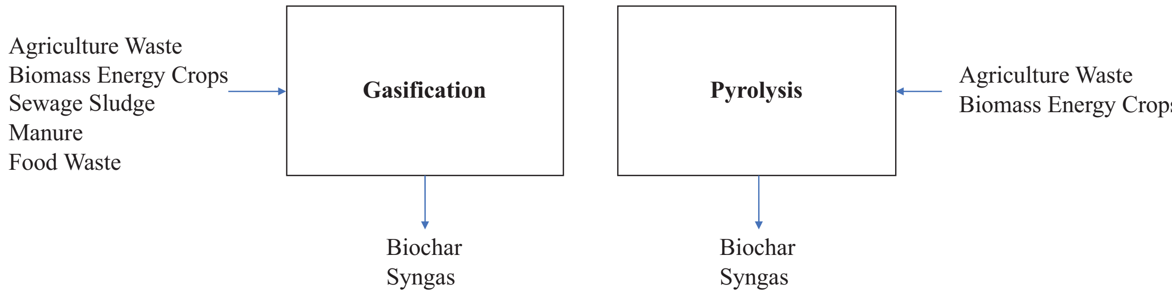


**Fig. 1.** Biochar feedstock for different technologies

ucts such as urea and methanol. The results demonstrate that the stream biomass gasification is the best performing economic and environmental process pathway. Moreover, the methanol production route demonstrated the highest profit ($0.12 per kg of biomass input) with the minimum emissions (0.68 kg of $CO_2$-e per biomass input). Pourreza et al. (Pourreza Movahed et al., 2020) studied the environmental and economic objectives of an integrated solid waste management system considering anaerobic digestion, composting, and conventional landfilling.

From an EWF perspective, Al Ansari et al. (Al-Ansari et al., 2016) demonstrated the benefit of utilising biomass within the EWF nexus by harnessing energy from biomass waste to produce power, which is re-utilised within the system thus enhancing total resource efficiency. Tian et al. (Tian et al., 2018) optimised resource use efficiencies within the EWF nexus by capturing economic and environmental trade-offs. An agriculture case study was solved demonstrating that almost 60% decrease of fertiliser use could reduce national nitrogen yield and $N_2O$ emission by 50%. Luqman et al. (Luqman and Al-Ansari, 2020) developed a multi-generation system driven by renewable energy options such as solar and biomass derived energy considering various environmental conditions, and evaluated the energy and exergetic efficiencies. Karan et al. (Karan et al., 2018) explored the linkages within the nexus using a stochastic approach and a quantitative model, where the cost of sustainable EWF systems was estimated. The results indicated that the energy element of the nexus is the most significant component of the EWF system considered, representing approximately 86% of the total cost. Using decision making tools, Namany et al. (Namany et al., 2019) proposed an EWF Nexus approach to evaluate food security for a Qatar scenario. The study concludes that by diversifying the energy and water mix of the EWF nexus system through the introduction of more than 70% renewable energy technologies, and through the utilisation of reverse osmosis desalination, the environmental impact of the two sectors can be decreased by 60%. Bieber et al. (Bieber et al., 2018) developed a framework using the combination of an agent-based model and a mixed-integer linear model to optimise a power generation and water infrastructure system including the cost of food production. The results demonstrate that increasing carbon credit costs is only effective at very high values (approximately $100/t$CO_2$). In this case, the energy mix changes from natural gas and tends to biofuel and solar energies. Nie et al. (Nie et al., 2019) proposed an EWF nexus framework for land use optimisation to facilitate decision-making. Quantification of the framework explored the trade-offs and classified sustainable pathways for satisfying both human demands and natural conservation. Dhaubanjar et al. (Dhaubanjar et al., 2017) introduced an EWF framework that combines water and power system models that supports multi-objective optimisation problems using pareto fronts. Luqman et al. (Luqman and Al-Ansari, 2020) applied both energy and exergy efficiencies to access the overall performance of a proposed multi-generation system which captures EWF nexus dynamics. Similarly, Ghiat et al. (Ghiat et al., 2020) developed a thermodynamic model detailing an integrated bioenergy with carbon capture and storage (BECCS) system that is evaluated using overall energy and exergy efficiencies. Alherbawi et al. (Alherbawi et al., 2021) developed an EWF quantification model to evaluate and optimise biofuel production from the second-generation biomass. The model accounts for the energy, water and food requirement to produce 1 GJ of different biofuel products throughout their lifecycle. In addition, the model examines the overall EWF Nexus' balance by evaluating the system's ability to make up for exhausted resources (i.e., water), whereby, the energy requirement for the provisioning of an equivalent quantity of exhausted resources are evaluated through different "payback" scenarios.

Motivated by sustainable development, the concept of Eco Industrial Parks (EIPs) has gained widespread attention throughout many countries in order to improve the environmental performance of industries. In an EIP, different contributors share by-products, waste, and facilities to minimise the environmental impacts, while maximising their own profits. Therefore, the main objective of an EIP integration is to demonstrate that larger profits can be achieved through collaboration. Various case studies highlighting industrial interactions and collaboration mechanisms which aim to decrease the environmental impact can be found in the literature. A review of the literature concludes that most EIP studies focus on the provision of individual resources such as water and energy integration, Energy-Water (EW) and Energy-Food (EF) integration separately, rather than consider a collective EWF nexus approach that considers resource interdependencies. For instance, Lovelady and El-Halwagi (Lovelady and El-Halwagi, 2009) formulated a mathematical optimisation approach which integrates water sources such as wastewater among industries in an EIP. Taskhiri et al. (Taskhiri et al., 2011) developed an emergy-base mixed-integer linear programming optimisation model which minimises the emergy of the water network in an EIP. The model accounts for the water use, energy consumption and their environmental impacts. AlNouri et al. (Alnouri et al., 2015) developed a water superstructure using direct and indirect water use for an EIP which is solved by optimisation methods to determine the most cost effective design. Nair et al. (Nair et al., 2018) proposed a mixed-integer non-linear programming model that aims for simultaneous intra-plant and inter-plant heat integration. A centralised unit is designed for transport depending on the needs of sinks. Within EW integration, Fouladi and Linke (Fouladi and Linke, 2018) proposed an optimisation based model of sustainable industrial EW nexus integration for an EIP. Using a superstructure, the study captured the trade-offs between different sectors represented by a water treatment unit, desalination, and cooling systems. Ghazouani et al. (Ghazouani et al., 2017) developed a new model based on a previous MILP optimisation model, which considers the mass and heat recovery networks amongst multiple industrial plants with a set economic objective function. The study demonstrated that despite the significant increase in capitals costs, the EIP optimisation

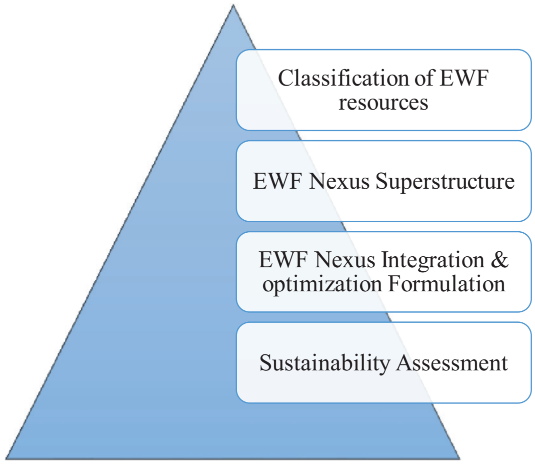


**Fig. 2.** EWF Nexus Methodology Steps.

can be profitable in different scenarios especially within saving the cooling utility requirements.

A review of the literature demonstrates that the application of the EWF nexus concept within industrial parks and the design of inter-plants has not been considered. Furthermore, despite the increasing methods and models, a unified framework, which integrates the EWF nexus as a whole and explores the trade-offs within an industrial setting is lacking. In addition, from the literature review, it can be concluded that the exergetic approach has not been applied to EWF nexus studies within industrial parks. As such, this study presents a novel superstructure and mathematical model which captures the synergies within EWF nexus considering interplants. It introduces a systematic approach to explore optimum designs for integrated water, energy, and food management, and to capture the trade-offs between the economic and environment dimensions of the problem. The multi-process system model developed in this study includes water production and treatment processes, ammonia/urea and GTL processes. These processes are simulated and optimised with respect to EWF nexus principles. The selection is driven by the fact that approximately 50% of the syngas produced is used in for ammonia production, 25% for hydrogen, and the remaining is utilised for Fisher-Tropsch products and others (Rauch et al., 2014). It is envisaged that biomass waste from the water treatment process and urban sector can significantly improve the resource efficiency of the selected processes and reduce the consumption of natural gas. In the next sections, a complete description on the methodology is provided followed by a case study.

## 3. Methodology

### 3.1. Overall synthesis approach

The main objective of this study is to manifest the energy, water and food nexus concept in an industrial network contributing towards the design and operation of eco-industrial parks, the methodological steps of which are outlined in Fig. 2. The industrial cluster considered in this study includes the GTL and Ammonia processes for which the performance of the overall system is enhanced through water integration and biomass utilisation. With the objective of enhancing resource efficiency, the optimisation model developed in this study includes a network superstructure encompassing the inter-linkages amongst EWF resources for the respective processes. In this study, the first law of thermodynamics in terms of energy is applied for the performance assessment. However, further integrating the second law of thermodynamics and exergy calculation captures the losses and inefficiencies more accurately. As such, this study adopts the exergetic approach (second law of thermodynamics) to compute the overall exergetic efficiency of the network, which is the ratio of the output's exergy content divided by the exergy content of the inputs. The exergetic efficiency is a more useful representation of work done and resource utilisation than standard energy efficiency calculations since it considers the real quality of the energy (Munir et al., 2014). The following sections describe the superstructure and the mathematical formulation of the optimisation network.

### 3.2. EWF nexus network superstructure

A network superstructure with different connections between resources is generated to ensure all different possible linkages are accounted for. In doing so, an existing water network problem has been expanded in order to consider agricultural and energy components (Alnouri et al., 2015; Alnouri et al., 2014). In this work, AlNouri et al. illustrated a representation of an industrial city to integrate water sources and sinks by using direct and indirect recycling integration plans with the objective of minimising the total annual cost. Results indicated that effective freshwater savings and waste minimisation using direct and indirect recycling can be obtained within the industrial city. In this study, the representation has been extended by adding the energy and agriculture sectors in order to integrate the potential for biomass utilisation into the network superstructure. Fig. 3 illustrates the elements for each sector of the network which are energy/water sources and sinks for a single plant. As illustrated in Fig. 3, the water sector is divided into process, treatment, and desalination units. Each unit is represented in terms of water and energy sources and sinks. Moreover, the food sector includes the agriculture and fertiliser elements. Based on regulations, the agriculture sector can only receive the freshwater produced from the desalination process. Treated wastewater can be used in any sink where the concentration of contaminants is within acceptable limits.

Fig. 4 represents the network design for two plants. Moreover, this study utilises biomass treated via the gasification process to produce syngas to generate power and offset a portion of the initial system energy requirements. Fig. 5 illustrates the nexus between energy and food sector via gasification process.

Given a set of source/sink data for water and energy; it is required to develop a systematic approach to determine the optimum network design with respect to the optimisation objective. The industrial city includes two process plants, treatment units, desalination units, and the food sector. The main objective of the network is to achieve the minimum total cost, which includes the costs of the production of freshwater, treatment of wastewater, energy, biomass gasification cost and is subjected to equality and inequality constraints. This is achieved by the simultaneous minimisation of the freshwater and energy consumption of the system.

$$Minimize : \left(C^{Freshwater} + C^{Treatment} + C^{Fuel} + C^{BiomassUtilisation}\right)$$

The "*what'sBest*" Mixed-Integer Global Solver for Microsoft Excel by LINDO Systems Inc is used to determine the global optimum solution. The following section describes the mathematical formulation of the optimisation.

### 3.3. Network optimisation mathematical formulation

The network optimisation is based on a mathematical formulation which includes the mass balances with contaminants inequalities for water sources and sinks in different units. As mentioned previously, a water network model developed previously (Alnouri et al., 2015; Alnouri et al., 2014) is used. The following

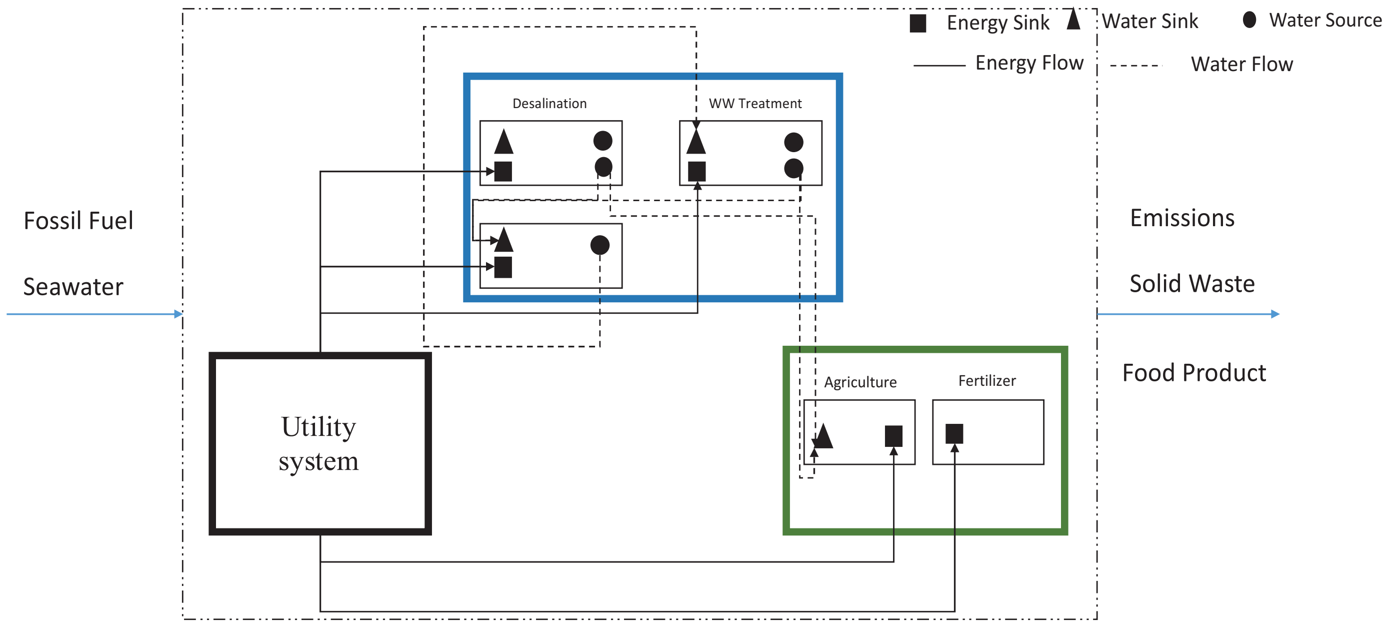


**Fig. 3.** Proposed EWF nexus superstructure-single plant.

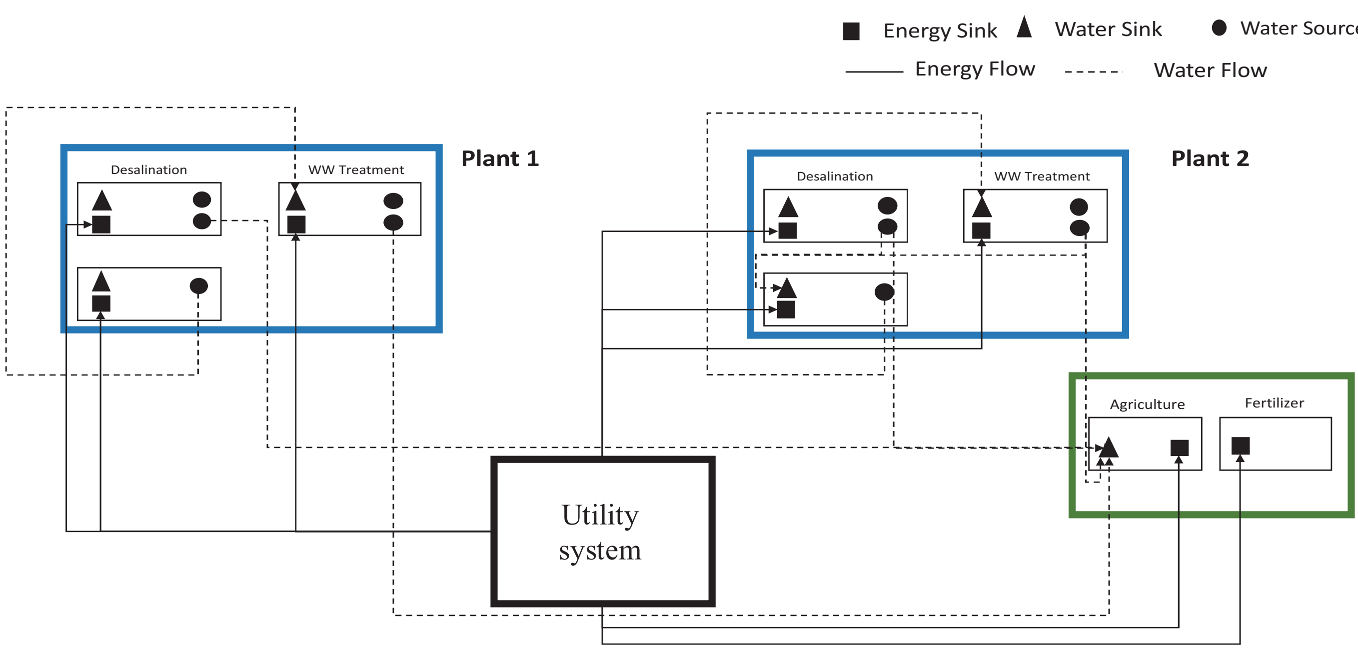


**Fig. 4.** Proposed EWF nexus superstructure-multiple plants.

equations summarise the main balances taken for the water network. The water source and sink balances and the contaminants are written as the following.

Water Source Balance:

$$\sum_{p,\ p\in P}\ \sum_{j\in SN_p} M_{ip,jp} + \sum_{s\in S}\sum_{t\in T} T^{Inlet}_{ip,st} + \sum_{s\in S}\sum_{t\in T} T^{Desalinaed}_{ip,st} + D_{ip} = W_{ip} \tag{1}$$

Water Sink Balance:

$$\sum_{p,p\in P}\ \sum_{i\in SU_p} M_{ip,jp} + \sum_{s\in S}\sum_{t\in T} T^{Treated}_{st,jp} + \sum_{s\in S}\sum_{t\in T} T^{Desalinated}_{st,jp} + \sum_{l\ \in L} F_{l,jp} = G_{jp} \tag{2}$$

Sink Contaminant Equality:

$$\sum_{p,\ p\in P}\ \sum_{i\in SU_p} M_{ip,jp} x^{Source}_{c,ip} + \sum_{s\in S}\sum_{t\in T} T^{Treated}_{st,jp} x^{Treated}_{c,st} + \sum_{l\ \in L} F_{l,jp} x^{FRESH}_{c,l} = G_{jp} z^{in}_{cjp} \tag{3}$$

Sink Pollutant Concentration Inequality:

$$z^{min}_{c,jp} \le z^{in}_{c,jp} \le z^{max}_{c,jp} \tag{4}$$

Moreover, the treatment units are designed and formulated using the recovery and removal ratios as illustrated below:

Treatment Balance:

$$\sum_{p\in P}\ \sum_{i\in SU_p} T^{Inlet}_{ip,sp} = \sum_{p\in P}\ \sum_{j\in SN_p} T^{Treated}_{rp,jp} + \sum_{p\in P}\ \sum_{v\in V} T^{Untreated}_{sp,vp}$$

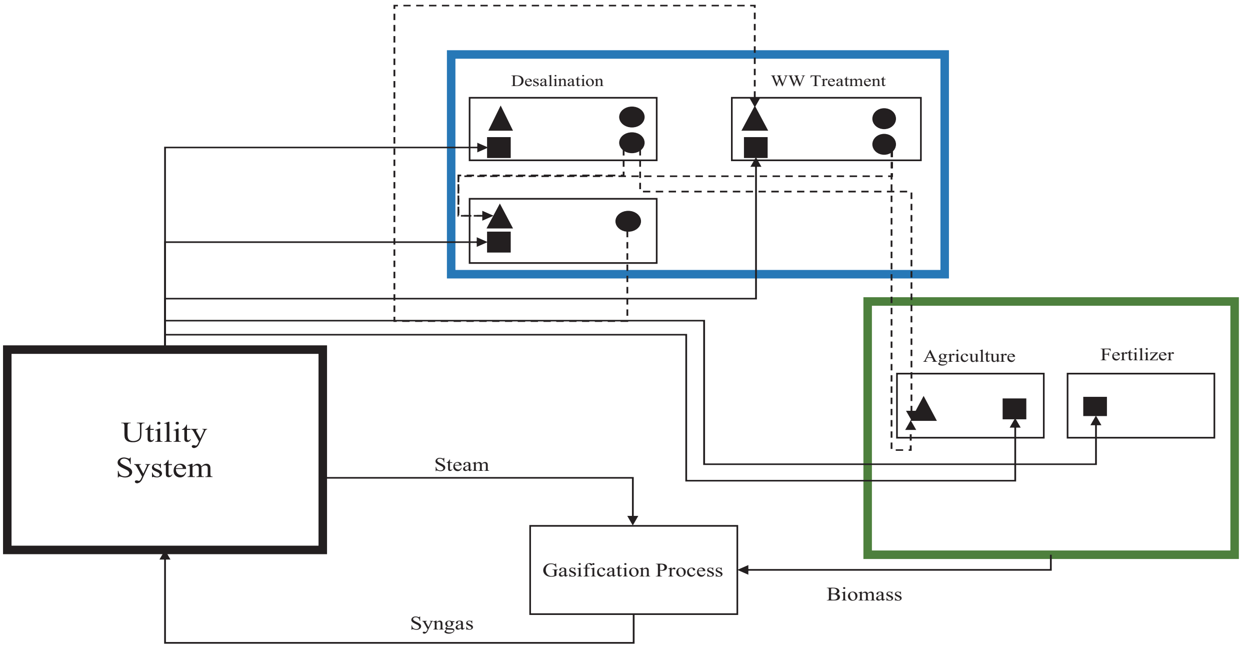


**Fig. 5.** Biomass Utilisation within EWF Nexus.

$$+\sum_{w\in W}\sum_{z\in Z}T^{Untreated}_{sp,wz}+D^{Treated}_{sp}+\ D^{Untreated}_{sp} \quad (5)$$

Treatment Recovery:

$$(1-\ R_{sp})\sum_{p\in P}\sum_{i\in SU_p}T^{Inlet}_{ip,sp}$$

$$=\left(\sum_{p\in P}\sum_{v\in V}T^{Untreated}_{rp,vp}+\sum_{w\in W}\sum_{z\in Z}T^{Untreated}_{sp,wz}+D^{Untreated}_{sp}\right) \quad (6)$$

Total Wastewater Discharge:

$$WW^{total}=\sum_{p\in P}\sum_{i\in SU_p}D_{ip}\ +\sum_{s\in S}\sum_{t\in T}D^{Treated}_{st} \quad (7)$$

Brine Discharge:

$$B^{total}=\sum_{s\in S}\sum_{t\in T}D^{Untreated}_{st} \quad (8)$$

Wastewater Discharge Load:

$$WW^{total}x^{WW\_Discharge}_{c}=\sum_{p\in P}\sum_{i\in SU_p}D_{ip}\ x^{Source}_{c,ip}+\sum_{s\in S}\sum_{t\in T}D^{Treated}_{st}x^{Treated}_{c,st} \quad (9)$$

Brine Discharge Load:

$$B^{total}x^{B\_Discharge}_{c}=\sum_{s\in S}\sum_{t\in T}D^{Untreated}_{st}x^{Untreated}_{c,st} \quad (10)$$

In the energy network model, the summation of all energy sinks must equal the energy source ($E_h$) which is provided by the utility system as illustrated in the following equation.

$$\sum_{p}E_{h,\ o}=E_h \quad (11)$$

Moreover, as mentioned previously, the concept of energy-food nexus in this study is fundamentally based on the biomass gasification process which produces syngas that can offset natural gas requirements. The energy-food integration is represented by mass and energy. An air-stream gasification model developed previously to produce $H_2$-rich syngas was utilised [AlNouss et al., 2018]. Using the results from the simulation, the following equation calculates the maximum syngas which can be produced from the biomass amount.

$$M_{syngasB,\ max}=XM_{Biomass} \quad (12)$$

Where X is the syngas to biomass ratio which is obtained from the simulation results. For each plant, the syngas produced from biomass should be equal or less than the required syngas for that specific plant. For example, for plant A;

$$M_{syngasB,\ A}\le M_{syngas,\ A} \quad (13)$$

$$\sum_{i=0}^{n}M_{syngasB,\ n}\le M_{syngasB,\ max} \quad (14)$$

After allocating the syngas produced from biomass to the different plant sinks, the flowrates of the natural gas required for those plants are recalculated using the syngas to natural gas ratios in the simulation (Y).

$$M_{NG,\ A}=(YM_{NG,\ A})-M_{syngasB,\ A} \quad (15)$$

### 3.4. Sustainability Indicators

There are multiple sustainability indicators and methods available related to economic, environmental, and social categories. Economic indicators involve minimising the total annual cost of the network. In terms of resource efficiency and environmental impact indicators, this study considers the following.

3.4.1 Global Warming Potential (GWP) Impact:

This indicator represents the impact of anthropogenic emissions which increase the radiative forcing of the atmosphere, causing the temperature of the earth's surface to increase. The GWP is computed through the following expression [Mosier et al., 2006]:

$$GWP=\sum_{j=1}^{j}m_j.EF_j \quad (16)$$

where j represents the elements, which contribute to the GWP, m is the flow rate of element j emitted (kg/FU) and EF is the emission

**Table 1**
Simulation data for selected plants [AlNouss et al., 2020].

| Flow rates (tonnes/d) | GTL | Ammonia |
|---|---|---|
| Natural Gas | 1.54E+04 | 1.54E+04 |
| Product | 1.03E+04 | 1.74E+04 |
| Wastewater produced | 1.90E+04 | 3.97E+04 |
| Process water requirement | 3.25E+03 | 6.23E+04 |

**Table 2**
Selected contaminants concentration [AlNouss et al., 2020].

| Wastewater Contaminants (ppm) | GTL | Ammonia |
|---|---|---|
| Total Dissolved Solid (TDS) | 2974 | 36.9 |
| Total Suspended Solids (TSS) | 4 | 0.264 |

**Table 3**
Environmental regulation [AlNouss et al., 2020].

| | TDS | TSS |
|---|---|---|
| **Discharge (ppm)** | 1500 | 46 |

factor of element j (kg $CO_2$eq./kg j). The elements considered in this work are $CO_2$, $CH_2$, and $N_2O$.

3.4.2 Exergy Efficiency:

The system's exergetic efficiency is defined in the following equation. In this study, the inputs considered are energy (Natural gas) and water flowing into the system [Fitzsimons et al., 2015].

$$Ex_{eff} = \frac{\sum_{j,p}(Products)}{\sum_{j,p}(Inputs)} \quad (17)$$

## 4. Illustrative Case Study

A case study of an industrial cluster of the selected processes in Qatar is presented to highlight the benefits of EWF nexus integration. The proposed approach is illustrated using a case study with two plants; Gas-to-Liquid (GTL) and Ammonia. Water data with selected two contaminants (TDS and TSS) is collected from a simulation in Aspen HYSYS. Different scenarios are solved by adding the agriculture sector to the case study and to complete the EWF nexus system. Table's 1 and 2 summarise the data used within the nexus problem.

Moreover, all wastewater discharging flows are satisfied by environmental regulations specified by the country as illustrated in Table 3.

For the Qatar case, this study integrates date palm residues (date pits), sewage sludge, food waste, and livestock manure into a process model representing the gasification process which includes the production of syngas (Table 4).

Therefore, using these data the nexus superstructure is integrated and solved using the "*what'sBest*" Mixed-Integer Global Solver for Microsoft Excel by LINDO Systems Inc. Using balances and indicators, multiple scenarios are solved as summarised in Table 6.

## 5. Results & discussion

The given case study in Section 4 has been optimised and simulated in different scenarios which are summarised in the following sections.

### *5.1. Scenario 1: Base case without any integration*

In the first scenario, the base case is solved without any energy-water integration intra or inter-plants. This scenario will be benchmarked against the other scenarios. All the water demand is satisfied by freshwater and the biomass waste management system is inactive. The best objective value obtained is approximately 1150 MM$ per year. Table 7 illustrates the simulation results of the solved scenario. Tables 5 and 8

### *5.2. Scenario 2: water network integration without biomass utilisation*

In this scenario, the water network is integrated without considering biomass management from the food sector (Figure 4).

#### *5.2.1. Case 1: Without wastewater reuse in agriculture*

Wastewater sources and the treated water cannot be used for the agriculture purposes due to the regulations in Qatar. After adding the water integration option, the total annual cost of the network is 1140 MM$ per year and Fig. 6 illustrates the optimum network design obtained.

As illustrated in Fig. 6, the wastewater sources from GTL and Ammonia plants are connected to the sinks in Ammonia or the treatment units. The total treated water is approximately 14800 tonnes per day which is sent to the Ammonia plant.

#### *5.2.2. Case 2: with wastewater reuse in agriculture*

For comparison purposes, another simulation is performed where the water sources from plants can be used within the agriculture sector. It is determined that the total annual cost of the network decreases by approximately 1% (1130 MM$ per year) since the flow rates of wastewater produced are very small compared to the agriculture sink requirement. Moving to the obtained network connection as illustrated in Table 9, the water produced in GTL plant is linked to the agriculture sink.

#### *5.2.3. Case 3: increase in wastewater reuse*

As demonstrated in the previous two cases, the impact of water integration is insignificant since the flow rates are small. In order to investigate this case, the wastewater sources are increased by a defined trend and the total annual cost of the network design is calculated. The wastewater sources flow rates from Ammonia and GTL plants are increased by 50 % and 100 % respectively. Fig. 7 demonstrates that larger flowrates of wastewater decreases the total annual cost of the network design as the treated water is cheaper than the desalinated water. Notably, the TAC can be reduced by almost 3.5 % by doubling the flowrates. This outcome indicates that water integration can be more significant for larger eco-industrial parks.

### *5.3. Scenario 3: EWF network integration with biomass utilisation – economic comparison*

Sewage sludge is the solid residual material which is formed as a by-product of the wastewater treatment plant. The produced sludge out of the treatment units can be added as the input to the biomass utilisation unit. In this scenario the biomass first comes from the closed system, which is the sludge produced from the treatment units in scenario 2. The energy substitution potential from biomass is assessed, where a similar observation to the second scenario is noticed. The network design and objective values are found to be the same, which indicates that the networks without biomass utilisation are more cost-effective. By breaking down the cost elements as illustrated in Table 10, it is concluded that the biomass utilisation is an expensive process and consequently the syngas produced from biomass has a much higher cost compared to natural gas combustion process, which is the case in scenario 1.

**Table 4**
Biomass feedstocks in Qatar [AlNouss et al., 2020].

| | Dried Sewage Sludge | Manure | Food Waste | Date pit waste |
|---|---|---|---|---|
| **Mass Flowrate (tonnes/y)** | $3.65 \times 10^4$ | $5.27 \times 10^5$ | $7.0 \times 10^3$ | $7.60 \times 10^3$ |
| **Ultimate analyses (wt %)** | | | | |
| N | 1.1 | 3.7 | 3.1 | 4.5 |
| H | 2.3 | 5.1 | 6.9 | 6.8 |
| C | 19.1 | 37.1 | 46.4 | 49.8 |
| O | 5.7 | 31.4 | 37.4 | 37.9 |
| Cl | 0 | 1 | 0 | 0 |
| S | 0.1 | 0.5 | 0 | 0 |
| Ash | 71.8 | 21.4 | 6.2 | 1 |
| **Proximate analyses (wt %)** | | | | |
| Moisture | 8.3 | 27.4 | 75.1 | 5 |
| Ash | 71.8 | 21.6 | 6.2 | 1 |
| Volatile matter | 8.8 | 65 | 86.1 | 81.8 |
| Fixed carbon | 19.4 | 13.5 | 7.7 | 17.2 |
| **LHV (dry basis) (MJ/kg)** | **20.5** | **19.4** | **19.12** | **34.07** |

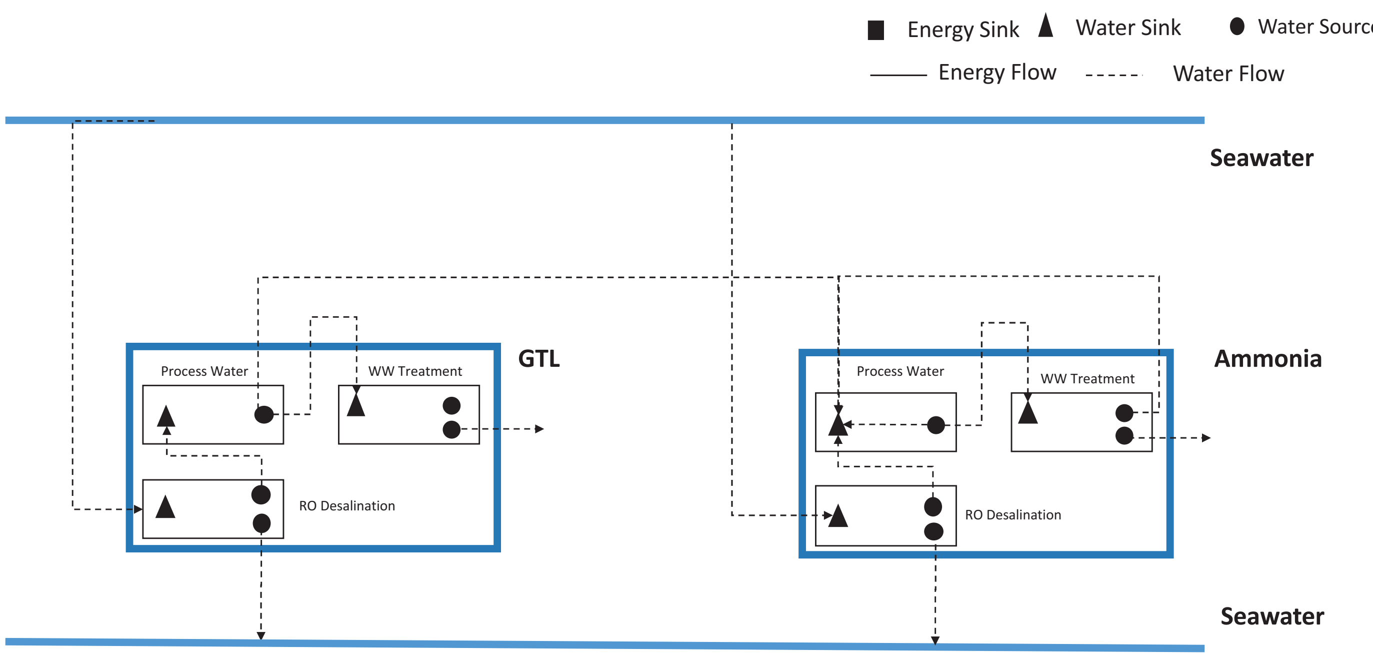


**Fig. 6.** Obtained network design of Scenario 2, case 1.

**Table 5**
Resource costs used in the simulation.

| | |
|---|---|
| **Freshwater Cost (\$/tonnes)** | 1.479 |
| **Energy Cost (\$/MMBTU)** | 2.27 |
| **Biomass Cost (\$/tonnes)** | 6.23 |

**Table 7**
Simulation results-scenario 1.

| | |
|---|---|
| **Freshwater (MMTonnes/d)** | 2.13 |
| **Total Wastewater Discharge (Tonnes/d)** | 58680 |
| **Total Power (KWh/yr)** | 3.21E+09 |
| **GWP (MMT $CO_2$-eq/yr)** | 30.4 |
| **Exergy Efficiency** | 0.363 |

**Table 6**
Scenario descriptions.

| | |
|---|---|
| **Scenario 1** | Base case without any energy-water integration is solved with an inactive biomass utilisation option.<br>*Optimisation Objective: Min TAC* |
| **Scenario 2** | Water network integration is added to the problem without biomass utilisation<br>*Optimisation Objective: Min TAC* |
| **Scenario 3** | Biomass utilisation option is activated in addition to water integration<br>*Optimisation Objective: Min TAC* |
| **Scenario 4** | Scenario 3 is solved by varying the optimisation objective<br>*Optimisation Objective: Min GWP* |
| **Scenario 5** | In this scenario the biochar produced is used to offset the urea need and reduce the ammonia production in the network design<br>*Optimisation Objective: Min TAC* |

**Table 8**
simulation results-scenario 2, case 1.

| | |
|---|---|
| **Freshwater (MMTonnes/d)** | 2.09 |
| **Total Wastewater Discharge (Tonnes/d)** | 0 |
| **Total Power (KWh/yr)** | 3.22E+09 |
| **GWP (MMT $CO_2$-eq/yr)** | 30.4 |
| **Exergy Efficiency** | 0.366 |

**Table 9**
Network sources-sinks connections.

| Source (tonnes/day) | Sink (tonnes/day) | | |
|---|---|---|---|
| | GTL | Ammonia | Agriculture |
| GTL | 0 | 2523.91 | 16472.09 |
| Ammonia | 0 | 8170.31 | 0 |

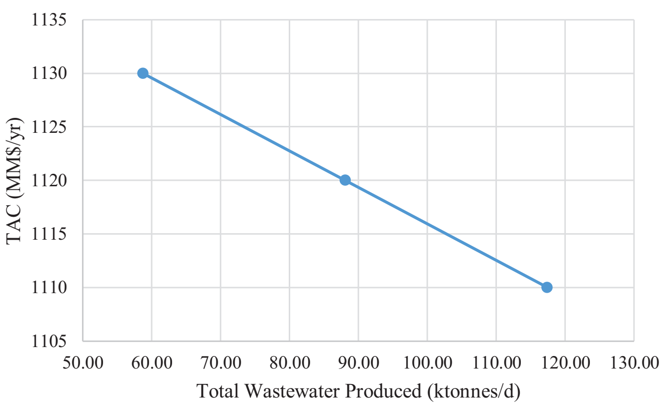


**Fig. 7.** Sensitivity analysis on wastewater flow rates.

**Table 10**
Cost elements of the network.

| | |
|---|---|
| **Freshwater (MMTonnes/d)** | 1.48 |
| **Energy Cost ($/tonnes)** | 0.078 |
| **Biomass Utilisation Cost ($/tonnes)** | 6.23 |
| **NG Price ($/MMBTU)** | 2.5 |

**Table 11**
Simulation results-scenario 4 with closed loop.

| | |
|---|---|
| **Freshwater (MMTonnes/d)** | 2.09 |
| **Total Wastewater Discharge (tonnes/d)** | 0 |
| **Total Power (KWh/yr)** | 3.22E+09 |
| **GWP (MMT $CO_2$-eq/yr)** | 30.2 |
| **Exergy Efficiency** | 0.367 |

### *5.4. Scenario 4: EWF network integration with biomass utilisation – environmental comparison*

As illustrated in scenario 3, with an objective for economic optimisation, the biomass utilisation option has been not selected within the network. Therefore, in order to evaluate the effect of biomass management system on the network in this scenario, the main objective is changed to the minimisation of the global warming potential, which also influences resource efficiency and implies the maximisation of the exergy efficiency as defined in section 3.4.2. As detailed in Table 11, the simulation results do not show significant change in the overall performance. The amount of solid waste out of the treatment units is neglectable with the closed loop.

Moreover, moving to an open loop system; as illustrated in Table 4, biomass such as food waste can be included from outside the defined system. In this case, the input to the biomass utilisation unit will be the sludge from the treatment units and the other waste sources in Qatar.

**Table 12**
Simulation results-scenario 4 with open loop.

| | |
|---|---|
| **Freshwater (MMT/d)** | 2.09 |
| **Total Wastewater Discharge (t/d)** | 0 |
| **Total Power (KWh/yr)** | 3.22E+09 |
| **GWP (MMT $CO_2$-eq/yr)** | 24.7 |
| **Exergy Efficiency** | 0.414 |

The simulation results demonstrate that the total annual cost of the network is approximately 3% more expensive than scenario 2 due to the expensive biomass utilisation unit. Table 12 and Fig. 8 illustrate the simulation results of the scenario and the network design superstructure, respectively. Comparing the results of different scenarios, it can be concluded that an increase of 3 % in the annual cost leads to a 18 % reduction in global warming potential. Furthermore, the exergy efficiency increases by approximately 5 percent.

As illustrated in Fig. 8, the syngas produced from biomass gasification process is sent to the GTL plant. Based on the simulation results, the GTL syngas to natural gas ratio is lower than that of Ammonia. Therefore, the syngas is used in GTL in order to decrease the natural gas usage.

Table 13 illustrates the comparison of different scenarios and biomass sources. It indicates that the utilisation of solid wastes generated from the treatment units and food sectors are able to result in more reduction in the GWP impact. The significant changes are achieved by having bigger industrial parks with more plants and larger sources as it is illustrated in the next sections.

Figure's 9 and 10 represents the comparison of different network elements for the all scenarios discussed earlier. The exergy efficiency trend in Fig. 9 illustrates that the efficiency almost remains constant throughout the first three scenarios, while in the last scenario it is increasing by 15 %. Replacing the natural gas by the syngas produced from the biomass gasification process, decreases the input material flow rates in the equation, which results in a higher exergy efficiency value. In addition, Fig. 9 illustrates the effect of adding the EWF nexus integration and the waste utilisation on the GWP. As discussed previously, the GWP remains constant until the final scenario and then reduces by approximately18 %. This is because the substitution of natural gas replacement removes the combustion emissions corresponding to its utilisation.

Finally, Fig. 10 indicates that the freshwater consumption decreases slightly after the water integration and optimisation in scenario 2 which is consistent with theory. However, in the last 3 scenarios, it remains constant and no more integration is obtained in the water network. In the last three scenarios, all the wastewater produced are treated and reused. This implies that all the wastewater streams produced from the two processes have been treated to the acceptable contaminant level ensuring its useability in other water sinks.

### *5.5. Sustainability metrics*

A sustainability metric is adopted in order to quantify the effect of different EWF footprints such as water, energy and wastes with respect to the economic benefits. El-Halwagi (El-Halwagi, 2017) introduced a metric referred to as the Sustainability Weighted Return on Investment Metric "SWROIM" of project $p$ and is expressed as below:

$$SWROIM_p = \frac{AEP_p}{TCI_p}\left[1 + \sum_{i=1}^{N\ indicators} w_i\left(\frac{indicator_{p,i}}{indicator_i^{target}}\right)\right] \tag{18}$$

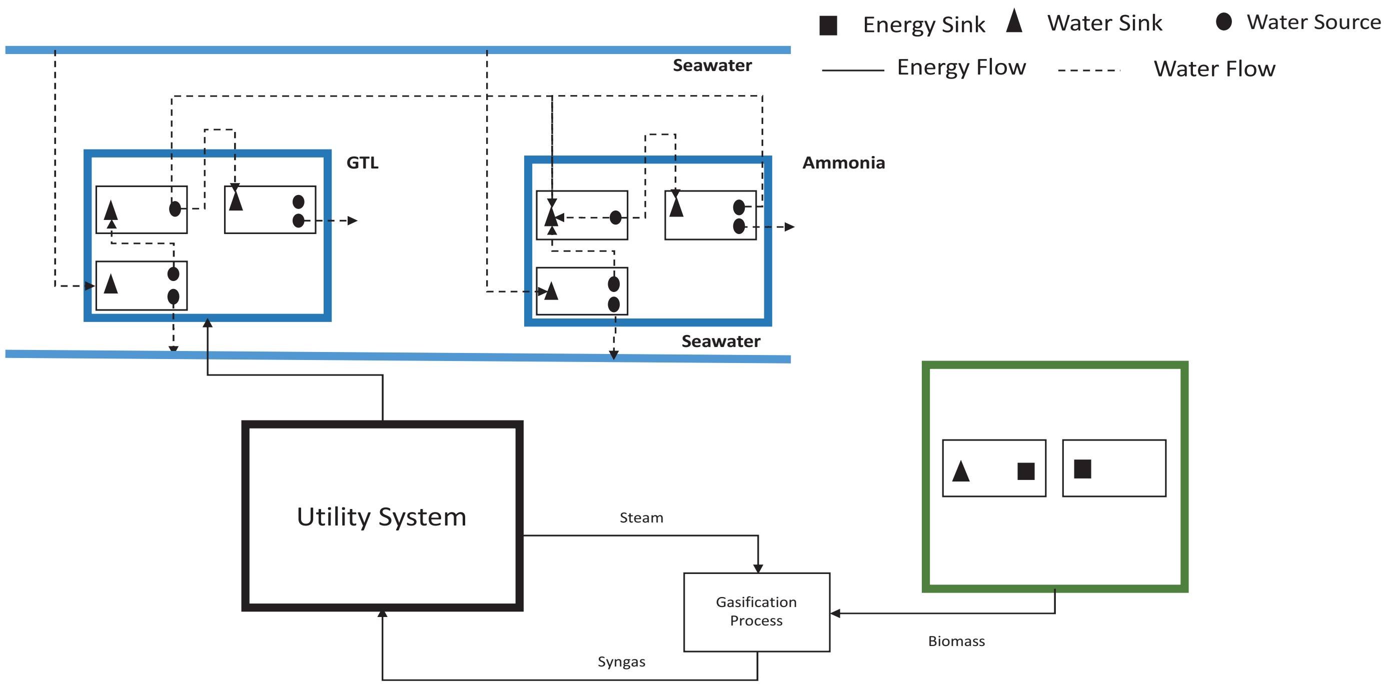


**Fig. 8.** Network design by Scenario 4.

**Table 13**
Simulation results-scenario 4.

| | Scenario 2 | Scenario 4-closed loop | Scenario 4-open loop |
|---|---|---|---|
| **Total solid waste (tonnes/yr)** | 1.82E+04 | 1.82E+04 | 5.96E+05 |
| **GWP (MMTonnes $CO_2$-eq/yr)** | 30.4 | 30.2 | 24.7 |

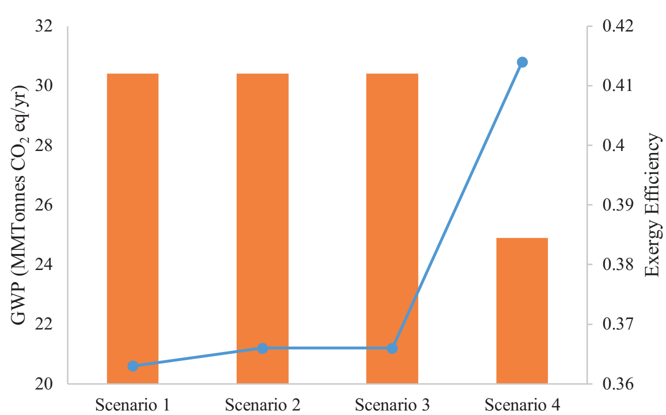


**Fig. 9.** Exergy Efficiency and GWP comparison of different scenarios.

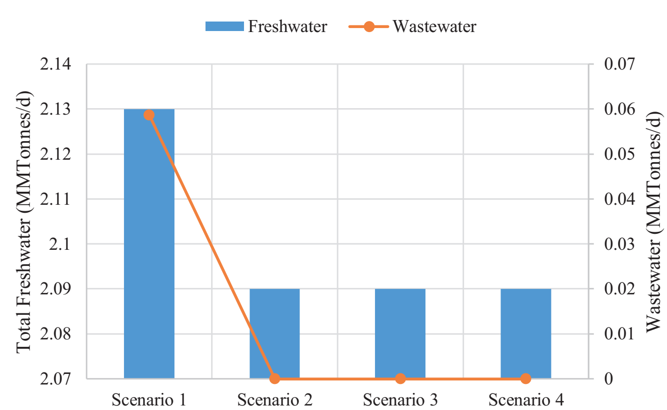


**Fig. 10.** water flow rates comparison of different scenarios.

**Table 14**
Relative importance of sustainability indicators for the case study.

| Sustainability indicator (i) | weighting factor ($w_i$) | Unit |
|---|---|---|
| Water footprint reduction | 0.25 | Kg/h |
| Solid waste reduction | 0.25 | Kg/h |
| Energy reduction | 0.25 | MW |

In the equation, AEP refers to the net annual economic profit, and the term TCI is the total capital investment of the project, where the ratio provides the return on investment (ROI). The index *i* is for any number of sustainability indicators aside from the net annual economic profit and *w* represents the weighing factor demonstrating the relative importance ratio of the $i^{th}$ sustainability indicator compared to the economic profit. Table 14 illustrates the sustainability indicators and their weighting factors used for the case study. All footprints are assumed to be equally weighted (0.25).

The sustainability metric (SWROIM) is computed for the four scenarios optimised. The results indicate that scenario 4 with open loop and represents solid waste utilisation is selected with the highest SWROIM value. The base scenario has the maximum SWROIM value which explains the lowest impact on sustainability. Table 15 and Fig. 11 illustrate the summary of the calculations and ROI/SWROIM results for the different scenarios.

The ROI and WROIM support decision making and implementation of the most sustainable scenarios. In order to further analyse the footprint reduction and to quantify the nexus, different val-

**Table 15**
Summary of scenarios with relevant indicators for the case study.

| Scenarios | TCI($) | AEP ($/yr) | Water reduction (kg/h) | Waste reduction (kg/h) | Energy reduction (MW) |
|---|---|---|---|---|---|
| **1** | 3.51E+08 | 6.51E+09 | -2.86E+05 | - | -3.21E+04 |
| **2** | 3.51E+08 | 6.51E+09 | -9.68E+05 | - | -3.22E+04 |
| **3** | 3.51E+08 | 6.51E+09 | -9.68E+05 | - | -3.22E+04 |
| **4-open loop** | 3.58E+08 | 6.51E+09 | -9.68E+05 | 4.84E+05 | -2.64E+04 |

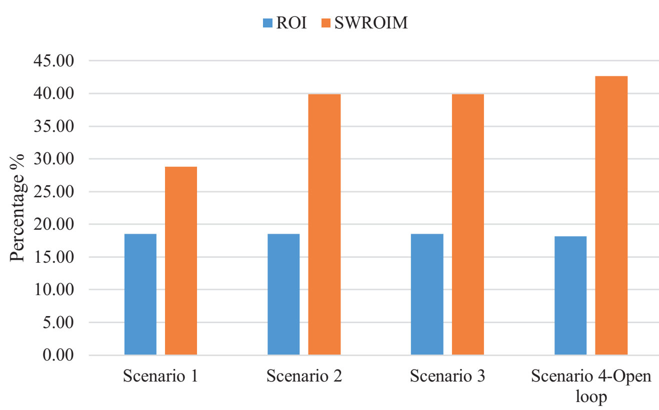


**Fig. 11.** ROI and SWROIM results for different scenarios.

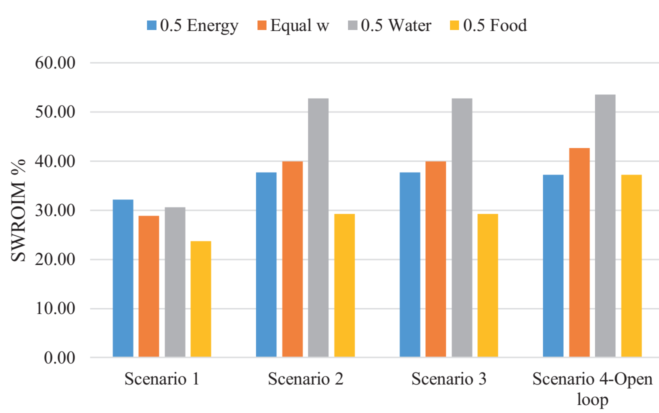


**Fig. 12.** SWROIM results for different weighting factors.

ues of weighting factors are used. The results in Fig. 12 support the biomass utilisation scenario as the most sustainable since the SWROM for all energy, water, and food sectors are the highest.

### 5.6. Ammonia replacement by biochar

Numerous studies have concentrated on the potential benefits of using biochar as a soil amendment. Since biochar offers better nutrient retention, it has gained significant attention as a possible replacement of conventional fertilisers, which in turn decreases environmental impacts. In this scenario, the biochar produced is used to offset the urea needed and reduces the ammonia production in the network design. In the literature, the ability of biochar to decrease the nitrogen fertiliser use is estimated at 10%-30% (Gaunt and Cowie, 2009). Scenario 4 with open loop and a reduction of 30 % has been used to calculate the biochar flowrate. As illustrated in Table 16, Ammonia replacement with biochar produced from biomass enhances the sustainability of the network in terms of emissions and the overall exergy efficiency. The GWP decreases by approximately 15 % due to the utilisation of a more environmentally friendly fertiliser alternative. Furthermore, the reduction of ammonia production leads to less natural gas as input and consequently a higher exergy efficiency.

**Table 16**
Scenario 5 results.

| | |
|---|---|
| **Biomass/Biochar Mass Ratio** | 0.248 |
| **Biochar (tonnes/d)** | 4.07E+03 |
| **GWP (MMTonnes $CO_2$-eq/yr)** | 20.3 |
| **Exergy Efficiency** | 0.464 |

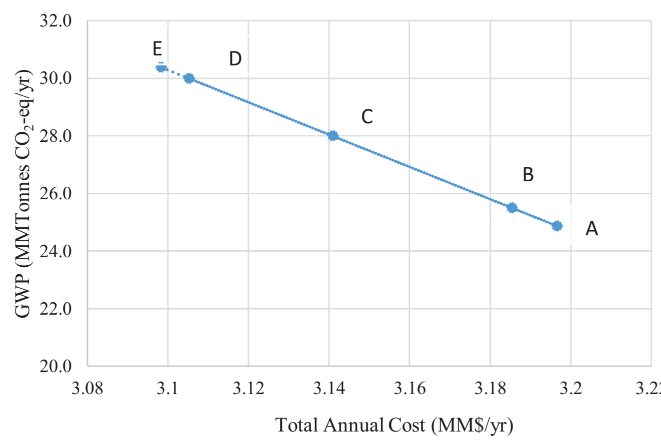


**Fig. 13.** TAC Vs. GWP pareto curve.

### 5.7. Multi-objectives optimisation problem

As discussed in the previous sections, the proposed optimised network has multiple objectives, which differentiates the network design. As such, it is necessary to develop an approach that captures the trade-offs between the economic and environmental metrics. In this work, the Pareto front curve is used for this purpose. First, the maximum and minimum GWP impacts of the proposed network are obtained by setting the optimisation objective to the GWP (as illustrated in scenario 2 and 4). Once these values are calculated, the optimisation objective changes to the economic objective, whilst there are constraints on the GWP impact. Fig. 13 is obtained using the maximum and minimum value for the GWP. Scenario A corresponds to the optimal economic solution, where the TAC is minimised, while scenario E corresponds to the optimal economic solution where the GWP impact has the minimum value. Scenarios B, C, and D are three intermediate points with the objective of total annual cost minimisation. It can be deduced that as the cost increases, the environmental impact decreases, which is reasonable and consistent with theory.

### 5.8. Energy price sensitivity analysis

To assess the performance of the network in various conditions, the effect of energy cost (natural gas price) is investigated based on the price in different countries. Table 17 illustrates the effect of the energy cost on the GWP impact. It is observed that the natural gas price range does not have any impact on the GWP of the network and the network design.

**Table 17**
Natural gas price for selectivity analysis.

| | Case 1 | Case 2 | Case 3 | Case 4 | Case 5 | Case 6 | Case 7 |
|---|---|---|---|---|---|---|---|
| **NG Price ($/MMBTU)** | 1.96 | 3.96 | 5.76 | 7.8 | 10.1 | 11.93 | 13.42 |
| **GWP (MMTonnes $CO_2$ eq)** | 30.4 | 30.4 | 30.4 | 30.4 | 30.4 | 30.4 | 30.4 |

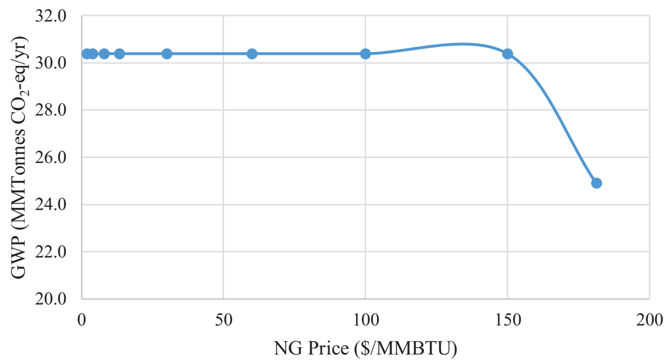


**Fig. 14.** Energy price sensitivity analysis.

This is because the biomass utilisation cost is much higher than the maximum cost for natural gas. Therefore, the network design does not change and consequently the energy consumption and GWP remains the same. However, the range of natural gas price is kept in order to identify the conditions in which the biomass utilisation option will be selected. Fig. 14 illustrates that at the price of almost 180 $/MMBTU of natural gas, the network design changes to the biomass utilisation case and the GWP is minimised.

## 6. Conclusion

This study developed a systematic approach for integration of industrial parks across the Energy-Water-Food nexus. A superstructure is generated which captures the linkages between different sectors. An optimisation formulation is used to capture the synergy potentials from water integration and solid waste utilisation. Moreover, the trade-offs between the economic and environmental metrics. In order to solve the multi-objective optimisation problem, the pareto front curve is generated. Noting that the biomass utilisation is an expensive process which is environmentally friendly, the results illustrate that the total annual cost minimisation scenarios do not select the biomass utilisation option. However, to minimise environmental emissions, a 3 % higher cost is added to the economic objective, which results in approximately 30 % reduction in the total GWP. Moreover, by reducing the resources utilisation, the exergy efficiency of the best scenario increased by 28 %. Furthermore, the sustainability metric (SWROIM) is used to quantify the nexus footprints. The results demonstrate that the scenario with biomass utilisation and open loop is selected with the highest SWROIM value. As such, this study demonstrates that the biomass utilisation has potential to reduce environmental impacts within EWF the nexus.

However, there are some limitations with the proposed algorithm. For instance, the limitation in the optimisation formulation can be in the non-linearity of the equations added. It becomes more difficult to identify a global optimum solution as non-linear equations increase. In this study, assumptions are added to the LINDO to reduce complexity. Moreover, the limitation in terms of modelling the eco-industrial parks modelling include distances between sources and sinks, safety, applicability, and control aspects of the problem. In future studies, integer decision variables will be added into the formulation. The superstructure can be expanded to create a hybrid EWF nexus and carbon network framework. Moreover, the implementation of multi-period framework and pipeline cost would enable the problem to be more accurate encompassing seasonal effects.

## 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.

## CRediT authorship contribution statement

**Jamileh Fouladi:** Conceptualization, Methodology, Software, Writing - original draft. **Ahmed AlNouss:** Conceptualization, Methodology, Software. **Tareq Al-Ansari:** Conceptualization, Writing - review & editing, Resources, Supervision, Project administration.

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