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Integrative design of the optimal biorefinery and bioethanol supply chain under the water-energy-food-land (WEFL) nexus framework

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A B S T R A C T S

This study presents a comprehensive decision model for the integrative design of a biorefinery for bioethanol production and its supply chain (BPSC) under the water-energy-food-land (WEFL) nexus framework. A new optimization model was developed using a mixed integer linear programming to simultaneously identify the optimal process configuration of a bioethanol production plant and the optimal bioethanol supply network. The objective function of the model is to minimize the total annual cost for establishing and operating the BPSC to meet society's needs (energy, water and food) under the limited resources and land availabilities, and technology capacity. The proposed model can provide the optimal solutions for design and operation of the BPSC: i) the types, and quantities of feedstocks; ii) types, number, and location of facilities and; iii) regional flows. The capability of the proposed model was validated through the case study of Jeju Island, Korea, with two scenarios: BPSC by cost (COPT) and nexus (NOPT) optimization. As a result, it was identified that the BPSC in NOPT requires higher energy supply cost (8.55 B$) than the COPT (6.44 B$). However, the BPSC in NOPT can satisfy the society demands with relatively smaller consumption of occupied land (2%), fresh water (30%) and primary energy consumption (64%) than that of the COPT, respectively.

1. Introduction

Global resources consumption is steadily increasing due to rapid population growth and socio-economic development [1]. Particularly, the drastic development of modern society has led to a tremendous increase in the demands for vital resources such as energy, food, water, and land, which has caused serious security issues for such resources. For instance, a Water Economic Forum report indicated that water scarcity has become one of the top five key issues over the past five years [2]. Meanwhile, agriculture is the largest water-consuming sector, which accounts for 85% of global freshwater consumption [2]. With increasing food demand, food production needs to be increased by 60% to satisfy the global food demand in the future, which will exacerbate the problem of water shortage [3]. In addition, bioenergy is regarded as one of the promising alternatives to meet increasing energy demand, while reducing the environmental impact (e.g., greenhouse gas emission) [4], despite of the conflict with the availability of land and water for food crops [5]. Therefore, to balance the increasing demand for these resources, these challenges should be addressed in a systematic way that simultaneously considers the interrelationships between land, water, food, and bioenergy, namely a resources nexus.

Considering these facts, the sustainability of bioethanol supply chain which involves land, water, energy, bioenergy as resources is very important. Some researchers proposed an optimization model to take the sustainability issues and their economic impacts into account for designing an optimal and sustainable bioethanol supply chain [6–9]. Ahranjani et al. proposed a hybrid multi-objective robust possibilistic programming model for sustainable bioethanol supply chain [6]. Akbarian-Saravi et al. proposed comprehensive decision approach to design and optimize sustainable bioethanol supply chain in which the bioethanol demand is predicted using an artificial neural network model [7]. Rabbani et al. developed an integrative optimization model for sustainable bioethanol supply chain considering the bioethanol production strategies [8].

The bioethanol supply chain within the nexus concept has been

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regarded as a powerful methodology for designing and managing a sustainable energy system [10–14]. Castillo et al. analyzed synergies and trade-offs of the biofuel production system under the land-water nexus framework [10]. Guo et al. proposed a multi-level system model for the bioethanol supply chain within the resource-food-bioenergy nexus [11]. Mahjoub and Sahebi developed a sustainable network design model for the water-energy nexus at the hybrid bioethanol supply chain [12]. López-Díaz developed an optimization model for bioethanol supply chain within water-energy-food nexus and analyzed trade-offs between the profit of system and the impact of uncertainties of strategic decisions [14].

Despite the large number of studies, there are still limitations in the application and interpretation of the nexus concept for integrative bioethanol supply chain which includes biorefinery, and energy supply system (e.g., water and food supply system). First, the complex interrelationships and interdependencies between the involved resources are still not clearly defined, which causes difficulties in the development and implementation of the nexus concept to real applications. One of the major reasons for the limited application of the nexus concept is that the practical benefits of using the nexus concept have not been proven yet. Most studies only focused on the efficient usage and supply of main resources and analysis of inter-resources competition. While these studies are helpful to understand the interactions between resources, they can neither provide adequate reasons for the incorporation of the resource nexus for designing real biomass-driven energy systems, nor explain the kind of benefits that can be expected from the economic and sustainable perspectives. Thus, to better understand the fundamental necessity for the consideration of the resource nexus, it is essential to quantitatively justify the benefits of the nexus-centric system by comparing with non-nexus systems.

Another limitation of the previous studies for resource nexus systems is the absence of dedicated models for a specific problem. For instance, the development of proper nexus models for a sustainable bioethanol supply chain can make the nexus concept more accessible and comprehensible by stakeholders and policy-markets [15]. In the sustainable bioethanol supply chain, the resource management using a nexus concept should encompass complex interactions and potential conflicts in all the stages, from biomass collection to bioethanol production and distribution. The design and management of the bioethanol supply chain under nexus framework should be expanded to also include other essential resources, activities, and disciplines such as land use, waste management, environmental impact, economics, resource efficiency, and ecosystem conservation to make the nexus even more multidimensional and interdisciplinary [16]. This is because such additional issues have become crucial in sustainable resource management, as resources are tightly interrelated and the use of one accompanies the presence of the others; e.g., the production of bioethanol requires water and land, which leads to a conflict with food as they compete with food crops on the use of agricultural lands and water, and the distribution of the produced bioethanol requires energy. While many approaches and models for the design of the bioethanol supply chain have been developed, no study comprehensively addresses all the problems that may arise in the bioethanol supply chain. Thus, proper resource nexus model for a bioethanol supply chain should provide specific and practical solutions for sustainable management such as biomass selection strategy, detailed bioethanol production strategies, and distribution scheme.

Therefore, the goal of this study is to propose a new optimization-based framework for the design and management of the resource nexus in the bioethanol supply chain, which can be used to address a wide range of issues such as i) understanding the complex interactions between the involved resources (i.e., synergy or trade-off) within the water-energy-food-land (WEFL) nexus, ii) identifying the optimal process configuration of a biorefinery and distribution strategies, and iii) evaluating the benefits and differences of the nexus-centric bioethanol system. To achieve this goal, the problem statement and system description are discussed in Section 2. We then develop an optimization model to identify the optimal design and management solution for the bioethanol supply chain using a mixed integer linear programming (MILP) technique in Section 3. Finally, we apply the proposed framework to a real case study, i.e., the nexus-centric bioethanol system in Jeju Island, Korea (Section 4), and discuss the major findings of the case study (Section 5).

2. Problem statement

The objective of this study is to propose a new integrative optimization-based framework for the design and management of a nexus-centric bioethanol supply chain. The developed framework should address the complexity of the interactions of all the related resources within the nexus, and provide practical solutions to a decision-making process, from biomass selection and biorefinery design to supply and distribution strategies. Thus, the problem addressed in this study can be described as follows:

- Given a certain region where a supply network of bioethanol is to be established.
- Given types of biomass along with potential cultivation land for satisfying the food and bioethanol demands. Note that two types of biomass are considered in this study: food crops and residues. While food crops refer to biomass that have already being grown, harvested, and utilized for food supply, residues refer to remnants of the biomass, which are lignocellulosic biomass (e.g., rice straw, barley straw, and beanstalk).
- Given different technologies that can be used in the biorefinery for bioethanol production.
- Given water availability to be used for different purposes (e.g., for agricultural and residential activities, and energy production).
- Given parameters of the involved elements, including biomass cost, land size, and cost required for biomass cultivation, water supply cost, technical and economic parameters of technologies (e.g., efficiency, capacity, investment, and operating costs), and costs for biomass and food crop transportation.

Note that a detailed explanation and values are given in Section 4. Based on the aforementioned conditions, the model can be simulated to determine the following decisions:

- Land-use strategy: location and size of the farmland.
- Crop cultivation: type, location, and quantity of the crops cultivated in the farmland.
- Water supply strategy: amount of water for farmland and social demands.
- Bioethanol production process design: process configuration of the biorefinery.
- Distribution strategy: size, number, and location of the involved facilities (e.g., warehouse and biorefinery). The amount of flows transported between region (e.g., biomass, food crops, bioethanol, and water) along with the corresponding transportation modes.

The assumptions made in this study are as follows:

- The system includes five nodes: farmland for food crop and residue production, warehouse (granary) for residue (food crop) storage, biorefinery, and water supply facility.
- There are no losses of food crop and agricultural residues during storage.
- The bioethanol is blended with gasoline using the existing infrastructure of the transportation sector such as terminal, oil refineries, and fuel stations; thus, no additional costs are incurred.
- All biomass resources and liquid fuels are transported between the nodes by truck.
- The market prices of the involved materials (e.g., food crop, biomass, bioethanol, and alternative products) are constant.

In this study, we generated two scenarios to comparatively analyze the effects of the WEFL nexus framework in the supply chain design of a bioethanol system. In the first scenario (COPT scenario), the optimal process configuration of the bioethanol production refinery as well as supply chain are determined from the economic perspective. Thus, the objective function is to minimize the cost for energy supply. As can be seen in Fig. 1 (a), bioethanol is produced from lignocellulosic biomass (i.e., agricultural residues) in a biorefinery and then distributed to satisfy the regional bioenergy demands. Thus, in the COPT scenario, the proposed optimization model is used to solve a typical allocation problem (i.e., optimal bioethanol supply chain), including the selection of types and amount of biomass, the technology configuration of the biorefineries, and the sizes and locations of the major facilities.

Comparing to the problem by the COPT scenario, the second scenario (NOPT) is created by adding the interrelationships between the resources (land, water, food, and bioenergy) as shown in Fig. 1 (b). In this nexus-centric bioethanol supply chain, two different feedstocks (food crop and agricultural residues) are supplied from farmlands. While the food crops are used to meet the social food demand of the involved region, the residues can be converted to bioethanol in the biorefinery to satisfy the energy demand. In this study, we consider three types of food crops: bean, rice and barley. Water sources should be supplied for three different purposes: for crop cultivation in the farmland, as utility in biorefineries, and to satisfy the regional water demands. The available land size for crop cultivation is restricted to a certain level, which is smaller than the actual land sizes of the involved regions. All types of agricultural residues (or food crops) are transported to biorefineries (or the involved regions) through warehouses (or granaries). Thus, the optimization model in the NOPT scenario identifies the optimal supply chain scheme to meet the water, food, and energy demands under a limited land size, which includes the type and amount of feedstock, the size and location of the major facilities, the number of transportation modes, and the regional distribution strategy.

Fig. 1 also shows the technology superstructure of the biorefineries for bioenergy production from lignocellulosic biomass. This study considered two technical pathways for biomass conversion in a biorefinery: biochemical and thermochemical pathways. Each pathway comprises several combinations of technologies and the corresponding energy or mass flows. As a feedstock for the biorefinery, this study considers three types of biomass: beanstalk, rice straw, and barley straw, which are the residues of major food crops. The lignocellulosic biomass is first decomposed into the two main intermediates (i.e., hydrolyzate and syngas by the biochemical and thermochemical pathway, respectively) through different types of pretreatment or gasification technologies. The amount and composition of the main intermediates depend on the types of biomass as well as the yields of the used technologies. Note that Fig. 1 shows alternative products such as electricity, hydrocarbons, and different alcohols. Excessive agricultural residues may often generate, when food is required for society needs and there is no energy demand. In this case, the excessive agricultural residues (i.e., lignocellulosic biomass) can be collected and converted to such alternative products for additional economic benefits by selling in a market.

In the biochemical pathway, the hydrolyzate produced by the pretreatment technology is converted to sugars, which is further processed for bioethanol production by the acidic or enzymatic saccharification and fermentation (*SSF*) technology. The produced raw ethanol is purified by stripping from the residues using the distillation or pervaporation technology. The separated residues can be combusted by the combined heat and power technology (CHP) to generate electricity or upgraded to value-added hydrocarbons (liquid fuels with hydrocarbons ranging from C5−C22) by the upgrading (UPG) technology, which is widely used in conventional refining industries, including thermal cracking, hydrocracking, and hydrotreatment processes [17]. Distillation (DTL) and pervaporation (PVL) technologies are used to purify ethanol from the fermented sugars. The syngas, which is a mixture of hydrogen and carbon monoxide obtained by the thermochemical pathway, is fed to the steam methane reforming (SMR) technology to synthesize only methanol or mixed alcohols (mixture of ethanol, propanol, butanol, and pentanol). The mixed alcohols are separated into ethanol and higher alcohols [18], whereas the methanol is converted into ethanol by a methanol-to-ethanol technology (MTE), which includes acetic acid synthesis and hydrogenation processes [19]. A more detailed explanation of the involved technologies can be found in literature [20,21].

3. Optimization model

The optimization model is formulated as a MILP problem. The following sections introduce the major constraints along with the objective function.

3.1. Constraints

3.1.1. Crop cultivation

Among the crops cultivated in region r, the total amount of biomass (F_{ir}) is calculated from each biomass produced per unit area (ε^F_{ir}) and the total utilized area in region r (A_r).

$$F_{ir} = \varepsilon^F_{ir} A_r \quad \forall i \in I^F,\ r \in R \tag{1}$$

The total amount of the food crop obtained from the crops cultivated in region r (G_{ir}) is given by:

$$G_{ir} = \varepsilon^G_{ir} A_r \quad \forall i \in I^G,\ r \in R \tag{2}$$

where ε^G_{ir} is the amount of each food crop produced per unit area in region r.

The land area utilized in region r cannot exceed the land availability of each region (ϖ_r), as follows:

$$\varpi_r \geq A_r \quad \forall r \in R \tag{3}$$

3.1.2. Distribution of biomass and food crops

The total amount of biomass obtained in region r is transported

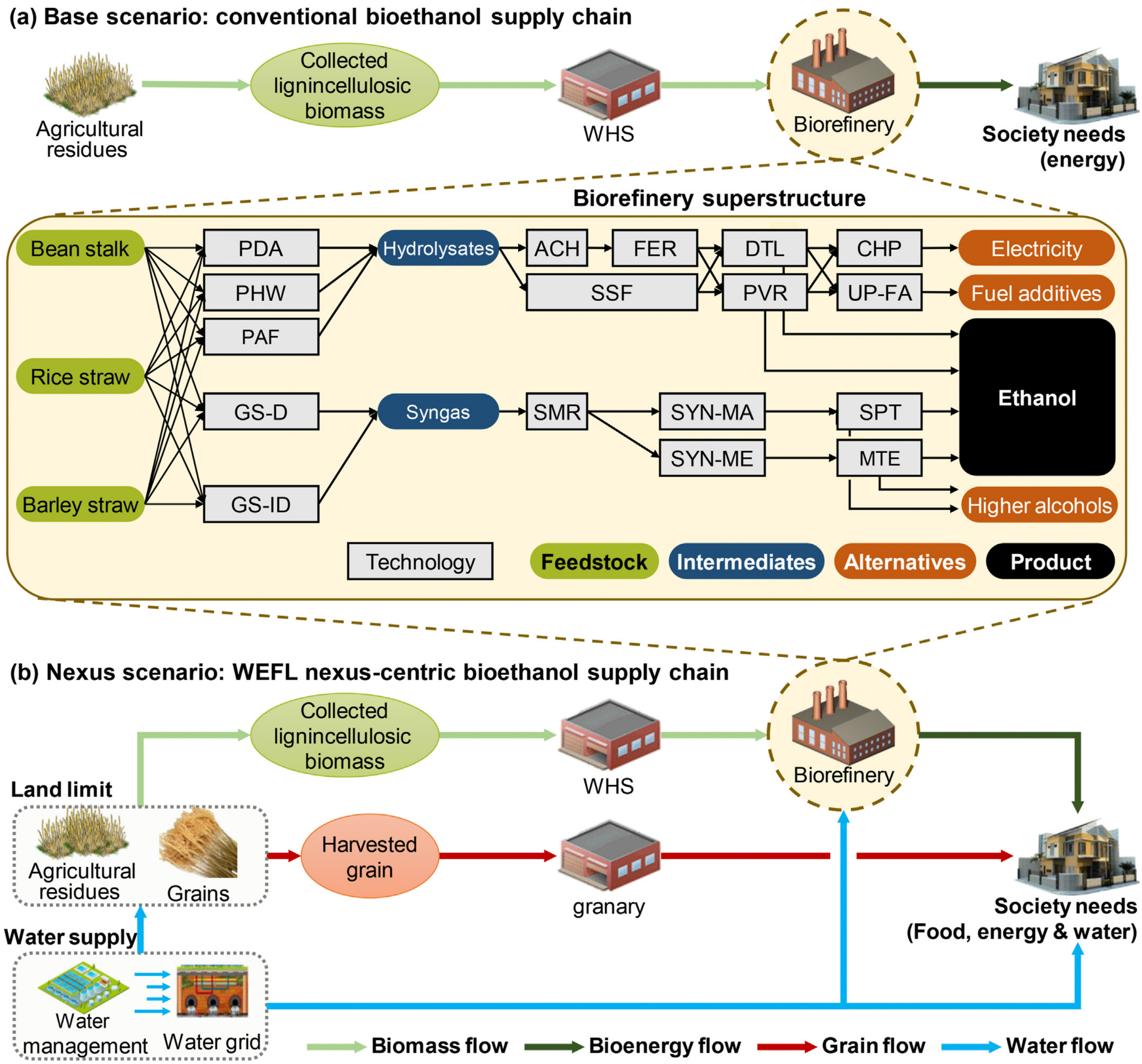

Fig. 1. Schematic representation of the bioethanol supply chains (a) without WEFL nexus and (b) with WEFL nexus, and the technology superstructure of a biorefinery. Abbreviation: PAF: Ammonia fiber expansion based pretreatment, PDA: Dilute acid based pretreatment, PHW: Hot water based pretreatment, ACH: Acidic hydrolysis, SSF-A: Simultaneous saccharification and fermentation using acid, SSF-E: Simultaneous saccharification and fermentation using enzyme, CHP: Combined heat and power generation, DTL: Distillation, PVR: Pervaporation, UP-FA: Upgrading to fuel additives, GS-D: Direct gasification, GS-ID: Indirect gasification, SMR: Steam methane reforming, SYN-MA: Mixed alcohol synthesis, SYN-ME: Methanol synthesis, MTE: Methanol to ethanol process.

to biomass warehouses.

$$F_{ir} = \sum_{r' \in R} Q^{FW}_{irr'} \ \forall i \in I^F, r \in R : r \neq r' \tag{4}$$

where $Q^{FW}_{irr'}$ is the flow rate of biomass transported from region r to the warehouses in region r'.

The total amount of biomass stored in the biomass warehouses in region r can be transported to the biorefinery in region r' and used to produce bioethanol.

$$\sum_{r' \in R} Q^{FW}_{ir'r} = \sum_{r' \in R} Q^{WP}_{irr'} \ \forall i \in I^F, r \in R : r \neq r' \tag{5}$$

where $Q^{WP}_{irr'}$ is the flow rate of the biomass transported from the biomass warehouses in region r to the biorefinery in region r'.

The total amount of food crops cultivated in a farmland in region r is transported to the food crop warehouses.

$$G_{ir} = \sum_{r' \in R} Q^{GW}_{irr'} \ \forall i \in I^G, r \in R : r \neq r' \tag{6}$$

where $Q^{GW}_{irr'}$ is the flow rate of the food crops transported from region r to the warehouses in region r'.

The food crops stored in the food crop warehouses in region r can be used to meet the food crop demand in region r'.

$$\sum_{r'\in R} Q^{GW}_{ir'r} = \sum_{r'\in R} Q^{WD}_{irr'} \ \forall i\in I^G, r\in R : r\neq r' \tag{7}$$

where $Q^{WD}_{irr'}$ is the flow rate of the food crops transported from the food crop warehouses in region r to meet the food crop demand in region r'.

3.1.3. Bioethanol production

The entire biomass transported to the biorefinery is used in biomass conversion facilities as an input material:

$$\sum_{r'\in R} Q^{WP}_{ir'r} = \sum_{j\in J^P} \eta^-_{ij} X_{ijr} \quad \forall i\in I^F,\ r\in R \tag{8}$$

where X_{ijr} is the amount of biomass processed by a facility, $j\in J^P$, in region r, and η^-_{ij} is a coefficient that indicates whether or not a facility, $j\in J^P$, can process biomass, $i\in I^F$ (1 if feedstock i can be processed by facility j, otherwise 0).

The total amount of intermediate products produced in all the facilities in region r should be processed by all the facilities within the region, as follows:

$$\sum_{i\in I^I}\sum_{j\in J^P} \eta^+_{ii'j} X_{ijr} = \sum_{j\in J^P} \eta^-_{i'j} X_{i'jr} \quad \forall i\in I^I,\ r\in R : i\neq i' \tag{9}$$

where $\eta^+_{ii'j}$ is the conversion efficiency of a facility, $j\in J^P$, which produces intermediate $i\in I^I$ from another intermediate $i'\in I^I$.

Eqs. (10) and (11) state the production of by-products and final product (i.e., bioethanol), respectively.

$$\sum_{i\in I^I}\sum_{j\in J^P} \eta^+_{ii'j} X_{ijr} = B_{i'r} \quad \forall i'\in I^B,\ r\in R \tag{10}$$

$$\sum_{i\in I^I}\sum_{j\in J^P} \eta^+_{ij} X_{ijr} = P_r \quad \forall\ r\in R \tag{11}$$

where $B_{i'r}$ and P_r are the total amounts of by-product and final product produced by all the facilities in region r, respectively.

3.1.4. Water supply

The overall water balance should be satisfied in the whole region. The sum of the amount of water supplied in region r should be equal to the sum of the amount of water consumed for three different purposes in the same region: i) to satisfy water demand (W^{FD}_r), ii) to operate a biorefinery (W^{FP}_r), and iii) to cultivate the crops (W^{FA}_r). The water supplied in region r comprises three types of water: underground water (W^U_r), tap water from the water supply system (W^T_r) and desalinated water ($W^D_{r'r}$).

$$W^U_r + W^T_r + \sum_{r'\in R} W^D_{r'r} = W^{FD}_r + \sum_{j\in J^P} W^{FP}_{jr} + W^{FA}_r \quad \forall\ r\in R \tag{12}$$

The amounts of water supplied as underground water and tap water in region r are respectively confined by the maximum amount, as represented by Eqs. (13) and (14).

$$W^U_r \le \lambda^U_r \quad \forall\ r\in R \tag{13}$$

$$W^T_r \le \lambda^T_r \quad \forall\ r\in R \tag{14}$$

Here, λ^U_r and λ^T_r are the availabilities of underground water and tap water from the water supply system in region r, respectively. Note that it is assumed that there is no limitation of amount of available desalinated water. The amount of water used in the farmland is calculated from the water required per unit production of the crops and the total amount of crops produced.

$$W^{FA}_r = \sum_{i\in I^F} \vartheta_{ir} F_{ir} \ \ \forall\ r\in R, \tag{15}$$

The biorefinery requires fresh water for its operation. The amount of water used in the biorefinery is determined by a conversion factor (ϕ_{jr}) and the amount of material produced by the biorefinery.

$$W^{FP}_{jr} = \sum_{i\in I^I} \phi_{jr} X_{ijr} \quad \forall j\in J^P, r\in R \tag{16}$$

3.1.5. Demand satisfaction

The food demands in region r should be satisfied by locally produced food crops in region r and food crops transported from region r' to region r.

$$PG_{ir} + \sum_{r'\in R} Q^{WD}_{ir'r} = \delta^G_{ir} \quad \forall\ i\in I^G, r\in R : r\neq r' \tag{17}$$

Here, PG_{ir} is the amount of produced food crops in region r.

The total amount of bioethanol produced in region r should be equal to the sum of the amount to meet the local bioethanol demand in region r (δ^E_r) and the bioethanol amount transported to another region r' to satisfy the energy demand of region r' ($Q^{PD}_{rr'}$).

$$P_r = \delta^E_r + \sum_{r'\in R} Q^{PD}_{rr'} \quad \forall\ r\in R : r\neq r' \tag{18}$$

The amount of water supplied to satisfy the water demand in region r should be equal to the water demand in the region.

$$W^{FD}_r = \delta^W_r \quad \forall\ r\in R \tag{19}$$

3.1.6. Capacity limitation

The total amount of energy and mass supplied to the biorefinery are restricted by the maximum capacity (χ^{max}_j) of the facilities. This limitation determines the number of facilities required, which is given as Eq. (20).

$$\sum_{i\in I} X_{ijr} \le \chi^{max}_j N_{jr} \quad \forall j\in J^P, r\in R \tag{20}$$

Similarly, the amount of mass stored in the warehouses is also restricted by the maximum storage capacity.

$$\sum_{r'\in R} Q^W_{ir'r} \le \chi^{max}_j N_{jr} \quad \forall i\in \left\{I^F, I^G\right\} I, j\in J^S, r\in R \tag{21}$$

3.2. Objective function

The objective function is to minimize the total annual cost (TAC), which is the sum of the total facility cost (TFC), total transportation cost (TTC), and total biomass cost (TSC), and minus the total byproduct credits (TBC).

$$Min\ TAC = TFC + TTC + TSC + TWC - TBC \tag{22}$$

The total facility cost is composed of facility investment cost and facility operation cost. The former is estimated by the unit investment cost of the energy production facilities and warehouses (φ_j) and the number of facilities installed (N_{jr}), while the latter is calculated from the unit operating cost of all the facilities (π_j) and the corresponding amount of energy produced or stored.

$$TFC = \sum_{j\in J}\sum_{r\in R}\alpha_j\varphi_j N_{jr} + \sum_{i\in I}\sum_{j\in J^W}\sum_{r,r'\in R}\pi_j\left(Q^{FW}_{irr'} + Q^{GW}_{irr'}\right) + \sum_{i\in I}\sum_{j\in J^P}\sum_{r,r'\in R}\pi_j X_{ijr} \tag{23}$$

where α_j is the capital charge factor for the amortizing investment cost of facility j.

The total transportation cost consists of the fixed (ν_i^{fix}) and variable costs (ν_i^{var}) of feedstock, food crops, and bioethanol, and the water supply cost.

$$TTC = \sum_{i\in I}\sum_{r,r'\in R}\left(\nu_i^{fix} + \nu_i^{var}2\varsigma_{rr'}\right) \times \left(Q^{FW}_{irr'} + Q^{WP}_{irr'} + Q^{GW}_{irr'} + Q^{WD}_{irr'} + Q^{PD}_{rr'}\right) + \sum_{r\in R}\left(\kappa^U W^U_r + \kappa^D W^D_r + \kappa^T W^T_r\right) \tag{24}$$

where $\varsigma_{rr'}$ is the distance between region r and region r'. Here, κ^U, κ^D, and κ^T are the supply cost of underwater, desalinated water, and top water, respectively.

The total biomass cost is composed of the rental cost of land that is utilized to cultivate biomass and food crops and the operating cost for obtaining biomass and food crop.

$$TSC = \sum_{i\in I}\sum_{r\in R}\varphi_r A_{ir} + \sum_{i,i'\in I}\sum_{r\in R}\left(\mu^F_r F_{ir} + \mu^G_r G_{i'r}\right) \tag{25}$$

where μ^F_r and μ^G_r are the operating cost for biomass and food crop, respectively.

The total byproduct credit is the additional profits obtained from selling the byproducts of the biorefinery (e.g. electricity or other chemicals), which can be produced in the biorefineries using extra feedstock after satisfying the energy demand:

$$TBC = \sum_{i\in I^B}\sum_{r\in R}\psi_i B_{ir} \tag{26}$$

4. Case study: application to Jeju Island, Korea

To illustrate the capabilities of the developed optimization model, we present a case study on the design of a nexus system in Jeju Island, Korea. This island is one of the best isolated regions to implement the bioethanol supply chain due to the abundance and variety of biomass for bioethanol production. Furthermore, the Korean government is actively planning to establish a sustainable and stand-alone energy system using only internal renewable resources, namely a carbon-free island. Thus, the introduction of bioethanol into the transportation sector can effectively improve regional independence and energy security since the energy demand of the transportation sector constitutes the major portion of the net primary energy consumption of Jeju Island [20,22].

4.1. Technology data of biorefinery

The technical and economic parameters of the major technologies used in the biorefinery and warehouses are summarized in Table 1. We considered two types of capacities (small and large) for all the facilities and used 0.6 as a scaling exponent to estimate the cost of facilities with different capacities [21,23,24]. Note that, for a particular technology, different types are considered according to the yield to process the same biomass or intermediates; however, we grouped them and used a single technical name (i.e., square boxes in Fig. 1) to simplify the system superstructure. For example, for the dilute acid-based pretreatment (PDA) technology that produces hydrolyzate from biomass, we considered three types of PDA technology with different yields. The detailed information of all the considered technologies are listed in Table S1 of the supplementary information.

To amortize the investment cost of the facilities, we assumed a capital charge factor of 0.1275 by considering an interest rate of 12% and a facility lifetime of 25 years [25]. For byproducts credit, the selling prices of electricity, hydrocarbon, and higher alcohols are considered as 1.13 $/kWh, 0.54 $/kg, and 0.56 $/kg, respectively [26–28].

For biomass and food crop transportation, we considered only a single transportation mode (i.e., the tank truck) because it is efficient in Jeju Island where the transportation distance is short and the demand variations between regions are huge [29]. The transportation cost of biomass and food crop consists of the distance fixed and variable cost, which are considered as 8.5 $/ton and 0.255 $/ton.km, respectively [20]. On the other hand, for bioethanol and water supply, only the distance variable cost is considered because bioethanol and water are assumed to be transported using the existing infrastructure. We considered 0.0512 $/ton.km for bioethanol, 0.085 $/ton for underground water, and 1 $/ton for the desalinated water [30,31].

4.2. Resource and geological data

We estimated the annual demands for water, bioenergy, and food in six regions of Jeju Island, which are shown in Fig. 2. Based on the renewable fuel standard policy of the Korean government, we assumed E3 (bioethanol 3% blend with gasoline) as the bioenergy demand. To estimate the bioenergy demand, statistical data such as fuel consumption, the registered number of vehicles, and the population of the six regions were used. For water and food demands, we used the regional population and the average values of water and food consumption per person.

The available amount of agricultural residues from the existing farmland is shown in Fig. 3. Note that the utilization of agricultural residues as a feedstock for bioethanol production is limited to avoid conflicts with other purposes (e.g., livestock feed) and for ecosystem conservation [20]. The net availability of agricultural residues for energy production was assumed to be 24.5% of the gross residue amounts [32]. The detailed parameter used to calculate the three demands are presented in Tables S2–S8 in of the supplementary information.

The land and water availabilities considered in this study are listed in Table 2. The available land size to cultivate the three crops (i.e, rice, barley, and bean) is assumed to be the sum of the area used in the current and 20% of the marginal land that is not currently used for other purposes in residential, commercial, industrial and public sectors [20,33]. For the water resource, the underground water and tap water from the water supply system are considered by the regional characteristic of Jeju. In Jeju, agricultural and residential water are supplied from these water resources. Particularly, tap water is mainly used to prevent seawater penetration by the use

Table 1
Technical and economic parameters of major technologies in the biorefinery and warehouse; full information are available in S1 of the supplementary information.

	Input	Output	Yield[a] (kg/kg)	Capacity (ton/yr)		CAPEX (M$)		OPEX ($/ton)
				S	L	S	L	
PDA	Feedstock	Hydrolyzate	3.74	4.2	8.3	8.8	13.3	5.0
PHW	Feedstock	Hydrolyzate	4.91	4.2	8.3	3.7	5.6	3.8
PAF	Feedstock	Hydrolyzate	3.92	4.2	8.3	3.7	5.6	3.8
GS-D	Feedstock	Syngas	0.67–0.70	4.2	8.3	25.3	38.4	22.5
GS-ID	Feedstock	Syngas	0.47–0.49	4.2	8.3	11.3	17.1	8.0
SSF-A	Hydrolyzate	Broth	0.96–1.01	2.1	4.2	3.9	5.9	0.8
SSF-E	Hydrolyzate	Broth	1.03	2.1	4.2	3.8	5.8	14.6
DTL	Broth	Ethanol	0.02–0.08	2.3	4.5	1.0	1.5	75.7
		Leftover	0.09–0.27	2.3	4.5	1.0	1.5	75.7
PVR	Broth	Ethanol	0.01–0.05	2.3	4.5	19.6	29.7	151.2
		Leftover	0.10–0.26	2.3	4.5	19.6	29.7	151.2
CHP	Leftover	Electricity	0.24–0.65[b]	0.6	1.2	0.7	1.0	93.9
UP-FA	Leftover	Hydrocarbon	0.07–0.08	0.6	1.2	13.3	20.2	79.7
SMR	CH_4-rich	Syngas	0.54–0.63	3.0	5.9	17.2	26.1	25.9
SYN-MA	Syngas	Mixed alcohol	0.56	0.4	0.8	3.0	4.6	100.0
SYN-ME	Syngas	Methanol	0.68	0.4	0.8	11.3	17.2	61.4
SPT	Mixed alcohol	Ethanol	0.32	0.3	0.5	1.3	2.0	77.0
		High alcohol	0.8	0.3	0.5	1.3	2.0	77.0
MTE	Methanol	Ethanol	1.38	0.3	0.6	22.2	33.6	579.2
BWH	Feedstock	Feedstock	1.38	3.0	6.0	3.3	5.0	15.0
	Food crops	Food crops	1.38	3.0	6.0	3.3	5.0	15.0

[a] Some values are over 1 due to additional inputs such as makeup water, solvents, or enzymes.
[b] The unit is kWh/kg.

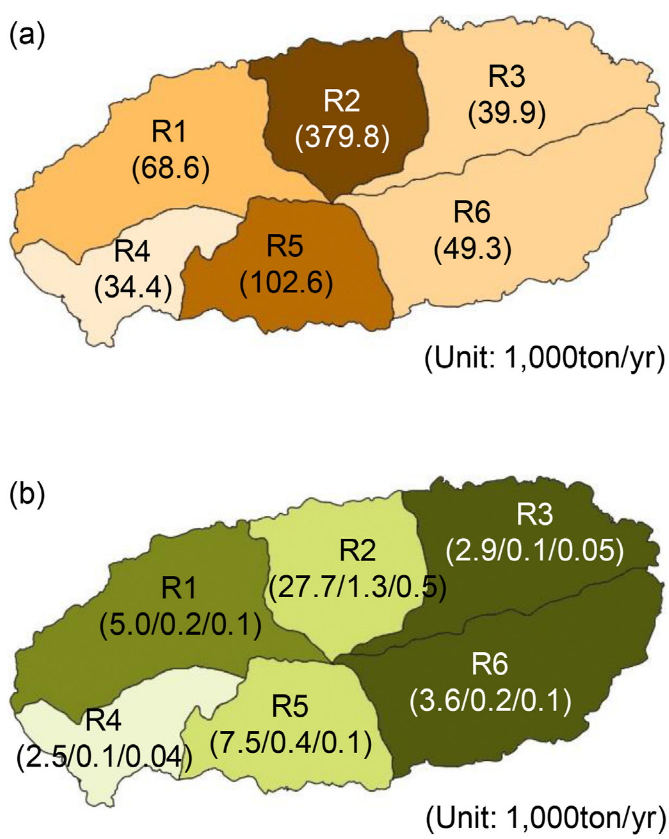

Fig. 2. Statistics of Jeju Island in 2014: (a) bioethanol demand in the road transport sector and (b) food demand (rice/barely/bean).

of a large amount of underground water. In this study, the usage rate of the tap water is assumed to be 7% of the use rate of underground water [22]. Based on a report on the water sources of Jeju [34], we assumed that water availability is 60% of the current usage for the sustainability of water sources. If the amount of water required in the nexus system exceeds the water availability, the excess water is assumed to be supplied by a desalination process.

We determined the total amount of crops produced in the farmland from the parameters related to the production of each crop per unit area and the regional production ratio of the crops [35]. The food crop part of the crop is supplied to satisfy the food demand, while the residue part is used to produce bioethanol as biomass. To calculate the amounts of food crop and biomass obtained from a crop, we considered the ratio of biomass to food crop (B/G ratio) [14,36]. Of the total amount of biomass obtained from each crop, some portion of biomass should be left on the farmland to minimize soil erosion and nutrient losses (e.g., organic matter, phosphorus, and magnesium) [37]. We assumed that only 95% of biomass can be used and the other 5% should be left in the farmland [37]. In addition, to determine the water consumption for crop cultivation, we considered the parameters related to the amount of water required to produce 1 kg of each crop. The detailed agricultural parameters such as crop yield, B/G ratio, and water requirement for growing each crop are summarized in Table 3 [38].

5. Optimization results

5.1. Optimal configuration for biorefinery

We applied the proposed optimization model to the design problem to identify the optimal configuration of biorefinery (e.g., the type of pretreatment technology, fermentation technology) and supply chain (e.g., mass and energy transportation between each regions). The selected technologies and their combination for the optimal biorefinery configuration in two scenarios are shown in Fig. 4. Both scenarios utilize three residues as feedstocks to produce bioethanol using four technologies sequentially. Hydrolyzate in the COPT scenario is synthesized by a hot water-based pretreatment (PHW) technology, whereas that in the NOPT scenario is produced by the PDA technology. While the COPT scenario considers only the energy flows without water flow, the NOPT scenario includes the water flow. The PHW technology is based on hot water; hence, it requires a large amount of water to process biomass. Therefore, in the NOPT scenario, the PDA technology, which does not use water

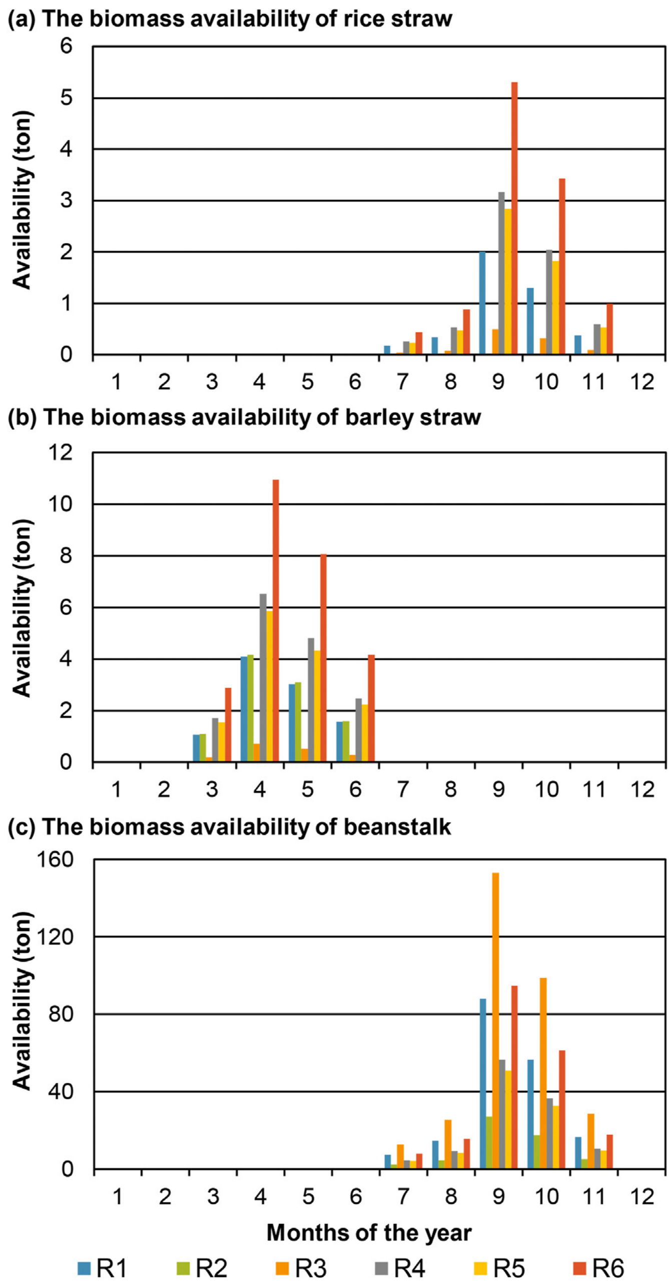

Fig. 3. Availability of agricultural residues for energy production from existing farmlands in Jeju Island.

Table 2
Land and water availabilities of six regions in Jeju Island.

	R1	R2	R3	R4	R5	R6
Land availability [km^2]	235	143	193	105	166	269
Land lease cost [$/$km^2$]	559	577	557	557	561	558
Underground water [10^3 ton/y]	617	460	690	294	716	1095
Tap water [10^3 ton/y]	44	241	25	22	65	30

as a utility, is selected to minimize the water consumption. The hydrolyzate produced by the PHW and PDA technologies in each scenario is then fermented and distilled into bioethanol. In addition, the dried residue is burned by the CHP technology to generate electricity as a byproduct.

5.2. Optimal biomass and bioethanol supply chain

The optimal strategies for land use and crop cultivation in the two scenarios are depicted in Fig. 5. For the COPT scenario, 129 km^2 and 252 km^2 of land areas are used in R3 and R6, respectively. Since the COPT scenario considers only bioenergy demand, a small amount of biomass is required and only two regions with the lowest land cost are used. Between the two regions, the land area used in R6 is more than twice of that used in R3 because of the greater land availability of R6. In the two regions, 12,000 tons of bean and 32,000 tons of rice are produced because of their relatively high efficiency for bioethanol production.

On the other hand, in the NOPT scenario, all the six regions are used to cultivate the crops. This is because the NOPT scenario includes food demand as well as bioenergy demand. Thus, large quantities of crops should be produced in the farmland considering the amount of food crop required to satisfy the food demand as well as the amount of biomass used to produce bioethanol. The total crop production in the NOPT scenario is about three times higher than that in the COPT scenario. Among the crops, since the food demand for rice is very high, the production amount of rice is the highest (107,206 tons). Among the six regions, R1 and R6 use the largest area of land (i.e., 235 km^2 in R1 and 269 km^2 in R6) because of the higher land availabilities of these regions.

The optimal supply network of the two scenarios is presented in Fig. 6. The thickness of the arrow indicates the quantity of the residues and bioethanol transported. The thicker the arrow, the greater are the amounts of energy and mass transported. As already seen in Fig. 5, in the COPT scenario, two types of residues (beanstalk and rice straw) are obtained in the two regions (R3 and R6) that have the lowest land cost. From these residues, bioethanol is produced in R3 and R6 and then transported to other regions to meet the energy demand. This is possibly because the COPT scenario is economically favorable over a centralized bioethanol production due to the low transportation cost of bioethanol. The amount of bioethanol produced in R3 from 11,655 tons of beanstalk is 4.4 ML/year, 78% of which is used to satisfy the energy demand of R2. R6 uses 32,112 tons of rice straw as biomass, produces 12 ML of bioethanol, and then transports most of it to R2. Most of the bioethanol is transported to R2 because the region has the highest amount of energy demand due to the largest population.

Unlike the COPT scenario, in the NOPT scenario, which additionally includes water and food demands, all the three types of residues are used to produce bioethanol (see Fig. 6(b)). In particular, the rice straw usage increased in the NOPT scenario to 59,101 tons, which is approximately 1.8 times of that in the COPT scenario. This is because the high food demand for rice increased the amount of rice cultivated in the farmland and the large amount of rice straw obtained from this is used to produce bioethanol as a feedstock. Unlike the COPT scenario, the NOPT scenario has a typical distributed network to minimize the total transportation cost. The NOPT scenario requires a significantly higher total transportation cost than the COPT scenario because of additional costs for food crop transportation and water supply. Thus, a biorefinery is installed in all the six regions. The bioethanol produced in the biorefinery of each region is first used to satisfy its own energy demand and then the remaining bioethanol is transported to R2.

Fig. 7 shows the food crop supply network from the farmland to food demand in scenario #2. For food crop storage, several food crop warehouses are built in all the six regions. The NOPT scenario requires a huge transportation cost due to water supply and biomass transportation as well as food crop transportation. Thus, the food crop warehouses are dispersively installed to minimize the food crop transportation between the regions. In the case of food crop transportation, the transportation of rice occurs more actively

Table 3
Agricultural parameters for crop cultivation.

	Production ratio (%)						Production amount per land area (ton/km^2)	Biomass/Food crop ratio	Water use (L/kg)
	R1	R2	R3	R4	R5	R6			
Rice	15	–	4	23	21	38	271	1.2	50
Barley	13	13	2	20	18	34	284	1.2	50
Bean	19	6	33	12	11	20	192	1.5	83

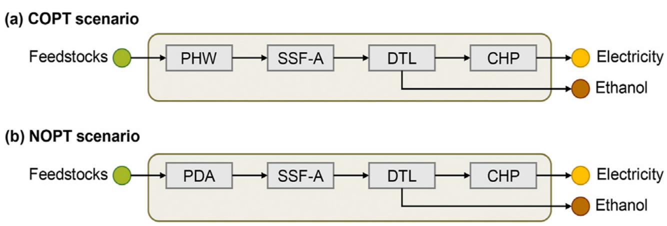

Fig. 4. Optimal technology configuration of the biorefinery in two scenarios.

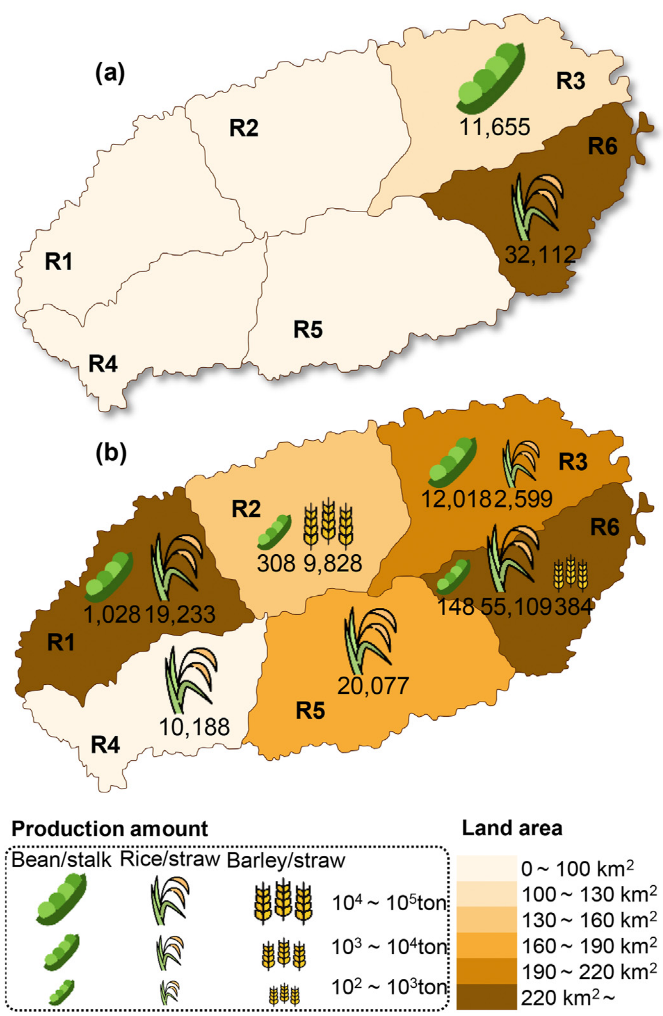

Fig. 5. Land-use strategy for the production of three crops in two scenarios: (a) the COPT, and (b) NOPT scenarios.

than that of the other two food crops. This is because the food demand for rice is overwhelmingly higher than that for the other two types of food crops since rice is Korea's staple food. Moreover, from the viewpoint of food crop distribution, most regions satisfy their own food demand from the on-site food crop warehouses. However, R2 meets its food demand by transporting the food crops from other regions. This is because R2, a major city on Jeju Island, has the highest food demand due to the largest population. However, since R2 has the highest land cost, it is more economical to transport the food crops from other regions than to build many on-site warehouses to store the food crops.

5.3. Effects of the WEFL nexus

The economics of the BPSC in two scenarios are compared in Fig. 8; the detailed cost information can be found in S9 of the supplementary information. Since the BPSC in the COPT scenario is established for energy supply, the cost breakdown includes only energy supply cost (green-colored components). On the other hand, the NOPT scenario include the food (yellow-colored) and water (blue-colored) supply costs as well as the energy cost.

It is first observed that the energy supply cost of the NOPT scenario is approximately 25% higher than that of the COPT scenario. Despite relatively high byproduct credits, the NOPT scenario requires large costs for capital, operating and raw materials compared to the COPT scenario, thereby resulting in high net energy supply cost ($684 M/year). Particularly, Fig. 8 shows a huge difference of the feedstock cost for energy production between two scenarios. Note that the feedstock cost for energy supply was simply calculated with total feedstock cost ($684 M/year) and the B/G ratio of the cultivated crops (see Table 3). For instance, the COPT scenario selected three types of the crops for food (bean, rice and barley) supply as shown in S10 of the supplementary information; accordingly, the corresponding residues (beanstalk, rice straw and barley straw) were used as a feedstock of energy production. Thus, the feedstock cost for energy production ($3.04 M/year) was proportionally calculated by B/G ratio of each crop over total cultivation cost ($5.51 M/year). And the rest ($2.47 M/year) were attributed to the feedstock cost for food supply.

In both scenarios, the facility investment cost was identified as the major cost drivers by accounting for 56.8% and 48.3% of the total energy supply cost, respectively. This is consistent with the general characteristics of the implementation of energy supply systems, which requires high investment costs.

Since the NOPT scenario, unlike the COPT scenario supplies not only energy but food and water, direct comparison of the economics of both scenarios is not instructive. Especially the synergy between energy and food supply in the WEFL nexus framework, such as decrease of occupied land and consumed water, was not observed. Therefore, to analyze the effects of WEFL nexus on the BPSC system, this study compares the water and energy consumptions, and land occupation for satisfying the social demands (i.e., water, bioethanol, and food). It was assumed that the land occupation for cultivating crops to satisfy food demand in the COPT scenario is calculated by the average of B/G ratio and production ratio. Detailed land use information can be found in S11 of the supplementary information.

Fig. 9 shows the water and primary energy consumptions, and

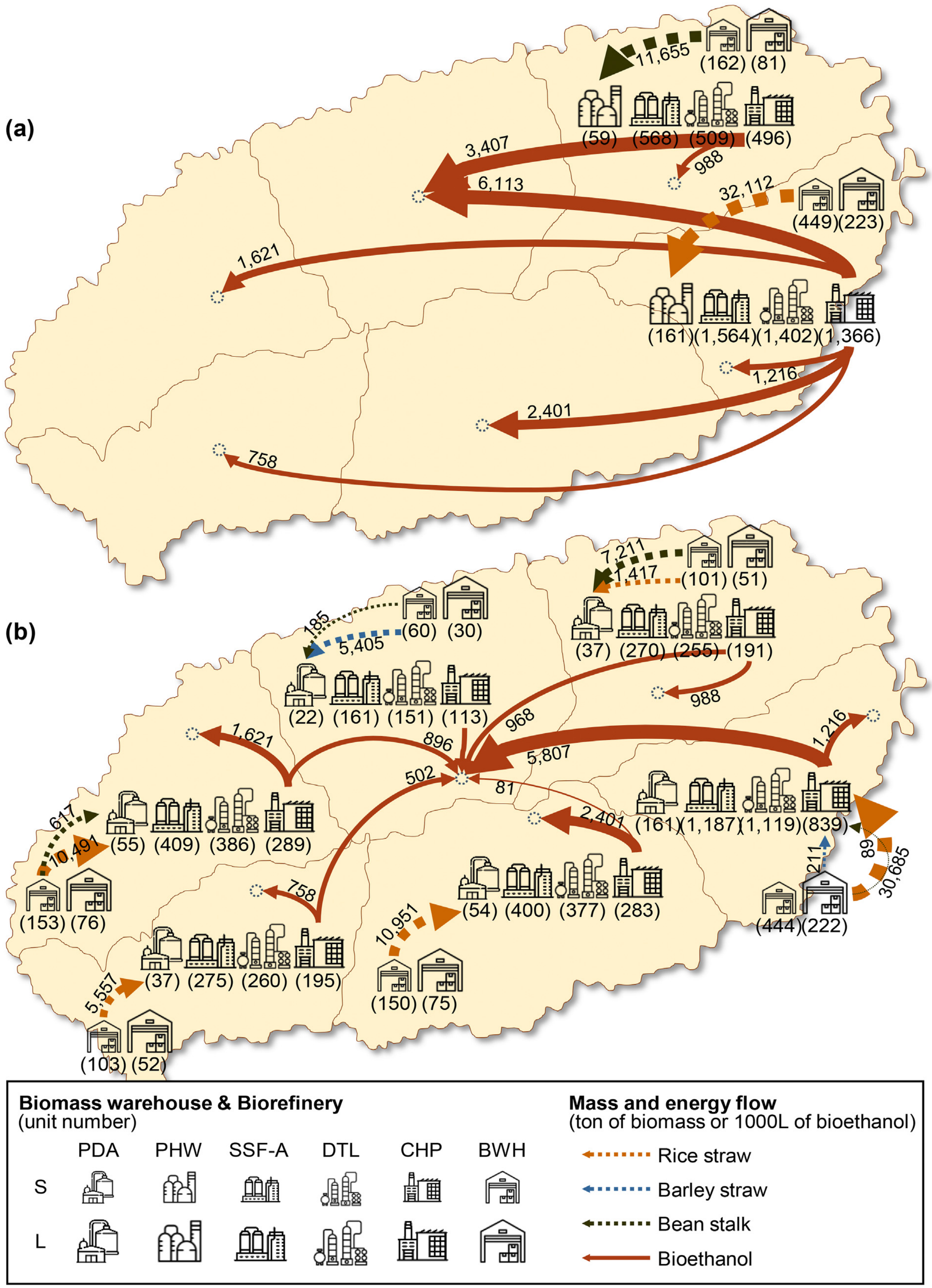

Fig. 6. Optimal configuration of energy supply network in two scenarios: (a) the COPT, and (b) NOPT scenarios.

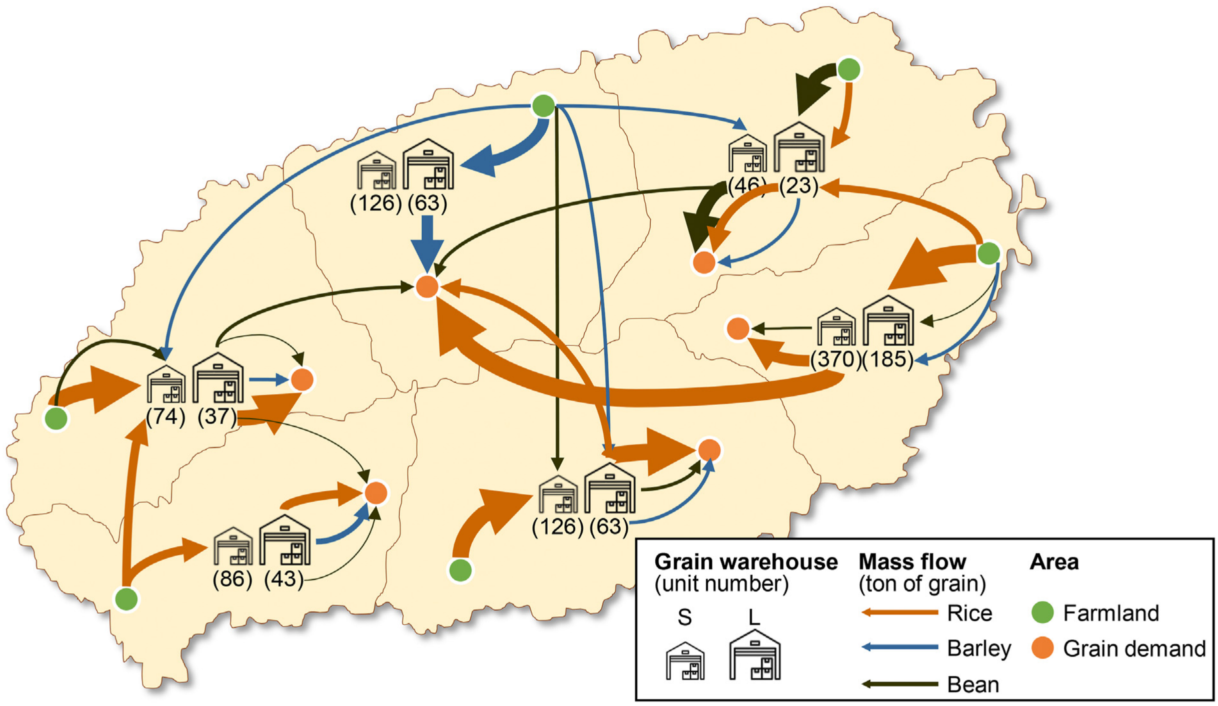

Fig. 7. Optimal configuration of food supply network in the NOPT scenario.

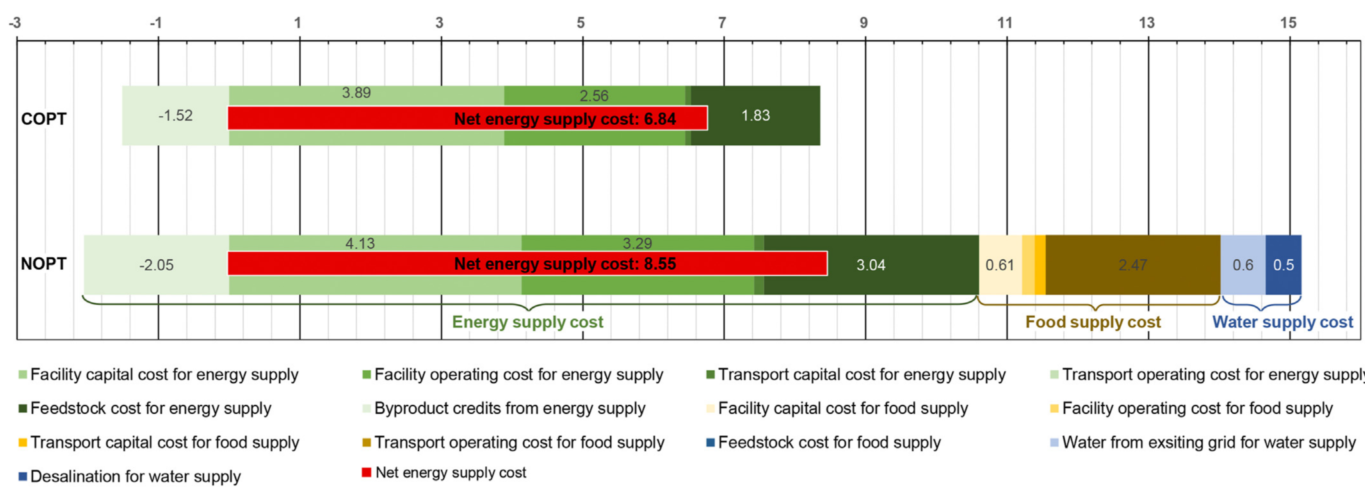

Fig. 8. Cost breakdown of the COPT and NOPT scenarios [100 M$/year].

occupied land size of two scenarios. The water consumption of the COPT scenario (18.1 GL/year) is approximately 30% more than the NOPT scenario (46 GL/year) mainly due to water consumption in the bioethanol production facility. The COPT scenario where the water availability is not considered, selected the PHW technology (biomass pretreatment using hot water) requiring huge amount of fresh water for an economic purpose. On the other hand, the PDA technology which pretreats biomass using a dilute acid was selected in the NOPT scenario to reduce water consumption. Selection of different pretreatment technologies yields different primary energy consumption rate in two scenarios. For instance, the energy consumption in the COPT scenario (516 TWh/year) is approximately 64% more than the NOPT scenario (315 TWh/year). Fig. 9 shows that total occupied land size of the NOPT scenario is less than the COPT scenario. In the COPT scenario, the optimal land size was determined to supply the lignocellulosic biomass for bioethanol production. On the other hand, the land occupation in the NOPT scenario was determined for both bioethanol and food supplies by identifying optimal crops types and quantities to suitably satisfying the social bioethanol and food demands of different-levels.

6. Conclusions

This study proposed a new optimization-based approach for the integrative design of a bioethanol production and its supply chain (BPSC) under the water-energy-food-land (WEFL) nexus framework. The developed optimization model minimized the total supply cost, which determines the supply network and allocation to the underlying system and is restricted by various practical and

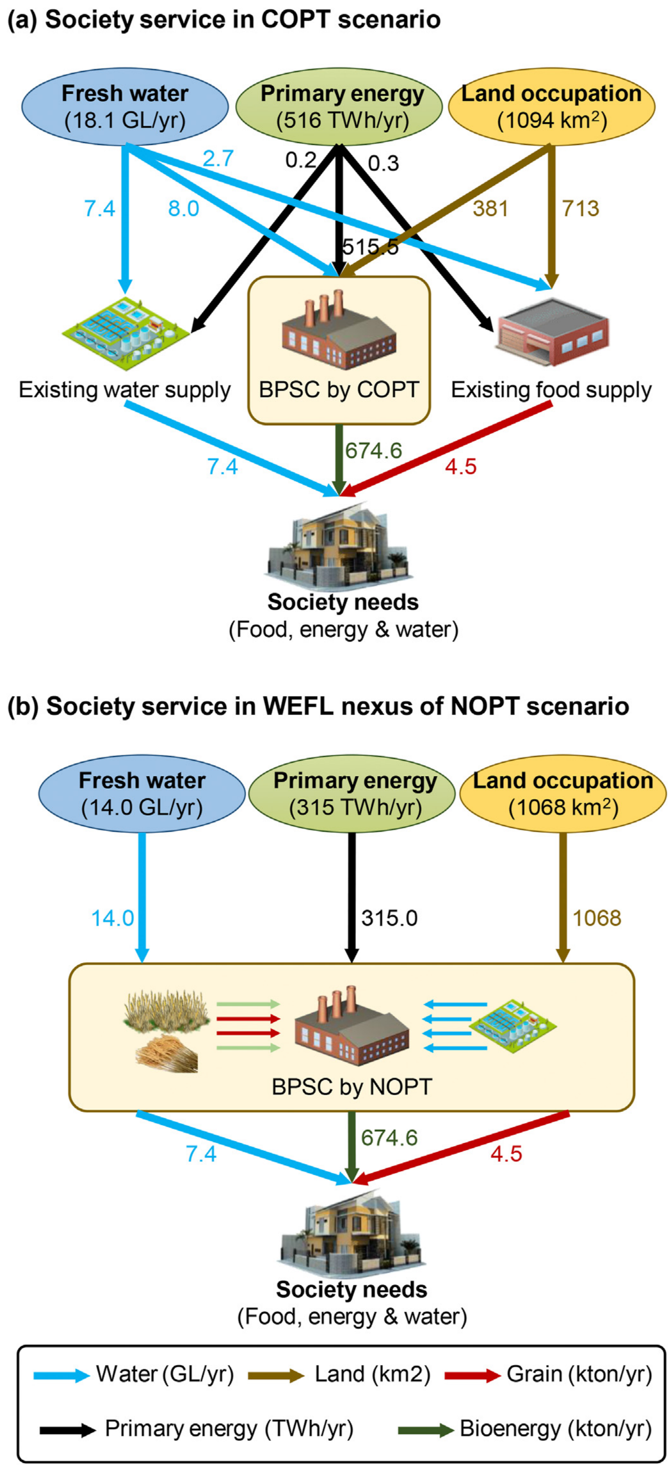

Fig. 9. Water and primary energy consumption, and land occupation to satisfy social demand in (a) the COPT and (b) NOPT scenarios.

logical constraints. In addition, we generated two design scenarios, cost minimization for bioethanol supply (COPT) and nexus optimization (NOPT), to illustrate the effect of the nexus system. The optimization model was applied to solve the design problem of bioethanol supply chain in Jeju Island, Korea, as a case study.

As a result, it was revealed that the optimal scheme of the biorefinery and bioethanol supply chain differs according to the design goal: cost vs. nexus perspectives. For instance, the hot water pretreatment (PHW) was selected in the biorefinery of the COPT scenario due to it low processing cost, whereas the NOPT scenario used the pretreatment technology using a dilute acid (PDA), instead of PHW, to reduce the use of fresh water. Accordingly, the BPSC in the NOPT scenario required higher energy supply cost than the COPT scenario to meet constant bioethanol demand. Furthermore, it was revealed that food, water and energy supply to a society in the WEFL nexus framework enables the BPSC to satisfy the society demands, with relatively small occupied land, fresh water and primary energy consumption.

The integrative approach to simultaneously design of biorefinery and supply chain in this study is useful to provide a comprehensive solution for planning of a sustainable bioethanol economy. Furthermore, this proposed approach can be further improved by securing detailed and precise parameters (e.g., resource availability, demand profiles and governmental policies), and considering different strategies such as dedicated energy crops, resource outsourcing and integration with existing energy industries. Furthermore, future research will include the following systematic techniques: the life cycle analysis (LCA) study climate change simulation to in detail assess the environmental impacts, multi-objective optimization to identify the tradeoff between core elements in the nexus system, and industrial ecology study for a wide range of applications (e.g., hydrogen economy or carbon dioxide (CO_2) utilization system) of the proposed approach.

Credit author statement

Seulki Han: Conceptualization, Writing-Original draft preparation Chanhee You: Visualization, Investigation, Writing – review & editing, Validation Jiyong Kim; Supervision, Project administration

Declaration of competing interest

All authors have no conflict of interest to declare.

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Nomenclature

Abbreviations

PDA	dilute acid-based pretreatment
PHW	hot water-based pretreatment
PAF	ammonia fiber expansion-based pretreatment
GS-D:	direct gasification
GS-ID	indirect gasification
SSF	simultaneous saccharification and fermentation
SSF-A:	acidic simultaneous saccharification and fermentation
SSF-E:	enzymatic simultaneous saccharification and fermentation
DTL:	distillation
PVR	pervaporation
CHP	combined heat and power generation
UPG	upgrading
SMR	steam methane reforming
S-MA	mixed alcohols synthesis
S-MM	mixed methanol synthesis
SPT	separation
MTE	methanol to ethanol
B/G ratio	ratio of biomass for energy to crop for food

WHS warehouse

Sets

I material
J facilities
R regions

Subsets

I^F biomass
I^G food crops
I^I intermediates
I^B by-products
J^W warehouse
J^P biorefinery

Parameters

ε_{ir}^F amount of biomass $i \in I^F$ cultivated from unit land area at region $r \in R$
ε_{ir}^G amount of food crop $i \in I^G$ cultivated from unit area at region $r \in R$
η_{ij}^- coefficient of facility $j \in J^P$ consuming biomass $i \in I^F$
$\eta_{ii'j}^+$ conversion efficiency of facility $j \in J^P$ which produces material $i \in I$ from material $i' \in I$
ϖ_r land availability of region $r \in R$
λ_r^U availability of underground water in region $r \in R$
λ_r^T availability of tap water in region $r \in R$
ϑ_{ir} amount of water required to cultivate 1 kg of each crop in region $r \in R$
ϕ_{jr} amount of water required to convert biomass through biorefinery $j \in J^P$ in region $r \in R$
δ_{ir}^G demand of food crop $i \in I^G$ in region $r \in R$
δ_r^E energy demand in region $r \in R$
δ_r^W water demand for living in region $r \in R$
χ_j^{max} maximum capacity of facility $j \in J$
φ_j unit investment cost of facility $j \in J$
φ_r unit land cost in region $r \in R$
π_j unit operating cost of facility $j \in J$
μ_r^F unit operating cost for biomass in region $r \in R$
μ_r^G unit operating cost for food crop in region $r \in R$
α_j capital charge factor of facility $j \in J$
ν_i^{fix} unit distance fixed cost of material $i \in I$
ν_i^{var} unit distance variable cost of material $i \in I$
$\varsigma_{rr'}$ distance between region $r \in R$ and region $r' \in R$
ψ_i selling price of byproduct $i \in I^B$
κ^U supply cost of underwater
κ^D supply cost of desalinated water
κ^K supply cost of topwater

Variables

A_r total land area utilized in region $r \in R$
$B_{i'r}$ amount of by-product $i \in I^B$ produced by all facilities in region $r \in R$
F_{ir} total amount of biomass $i \in I^F$ cultivated at region $r \in R$
G_{ir} total amount of food crop $i \in I^G$ cultivated at region $r \in R$
N_{jr} required number of facility $j \in J$ in region $r \in R$
P_r amount of final product produced by all facilities in region $r \in R$
PG_{ir} amount of produced food crop $i \in I^G$ in region r
$Q_{irr'}^{FW}$ flow rate of biomass $i \in I^F$ transported from region $r \in R$ to warehouse in region $r' \in R$
$Q_{irr'}^{WP}$ flow rate of biomass $i \in I^F$ transported from warehouse in region $r \in R$ to biorefinery in region $r' \in R$
$Q_{irr'}^{GW}$ flow rate of food crop $i \in I^G$ transported from region $r \in R$ to warehouse in region $r' \in R$
$Q_{rr'}^{PD}$ amount of final product transported from region $r \in R$ to region $r' \in R$
$Q_{irr'}^{WD}$ flow rate of food crop $i \in I^G$ transported from warehouse in region $r \in R$ to food crop demand in region $r' \in R$
TAC total annual cost
TFC total facility cost
TTC total transportation cost
TSC total biomass cost
TBC total byproduct credits
$W_{r'r}^D$ amount of desalinated water supplied from region $r \in R$ to region $r' \in R$
W_r^{FA} amount of water supplied to cultivate crop in agricultural land at region $r \in R$
W_r^{FD} amount of water supplied to satisfy water demand in region $r \in R$
W_r^{FP} amount of water supplied to operate a biorefinery in region $r \in R$
W_r^T amount of tap water consumed in region $r \in R$
W_r^U amount of underground water consumed in region $r \in R$
X_{ijr} amount of biomass $i \in I^F$ processed by a facility $j \in J^P$ in region $r \in R$

Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.energy.2021.120574.

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