Optimal Retrofitting of Conventional Oil Refinery into Sustainable Bio-refinery under Uncertainty

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Abstract

This paper focuses on a novel optimization problem to retrofit a conventional fossil-based refinery into a hybrid biomass-based refinery. A mixed-integer linear programming model, which considers a ten-year-long retrofit planning along with operational constraints in each year, is formulated. In addition to that, the problem is extended to a multistage stochastic programming model to handle both endogenous and exogenous uncertainties. The corresponding multistage problem is solved through a series of two-stage stochastic programming subproblems. Furthermore, a Lagrangean decomposition algorithm is implemented to solve such a problem. By determining whether to add new units or retrofit existing units to the selected biomass-based technologies, the results provide flexible design alternatives with consideration of operational constraints for each year. The results show the advantages of the selected biomass-based technologies and enhance the performance of the final solution under uncertainty.

Keywords: Refinery; Biomass; Retrofit; Stochastic programming; Lagrangean decomposition.

1 | INTRODUCTION

The Petroleum refinery industry, which has been regarded as the core supplier of fuels and carbon-based products over the last century, is now seeking a new opportunity to reduce carbon emissions and achieve sustainable development.[1] Biomass has been widely recognized as a promising renewable energy resource with great application potential. Instead of designing and constructing new infrastructure, an economically attractive option was proposed to retrofit an existing crude oil refinery into a biorefinery with certain technologies that can convert biomass into hydrocarbons. [2]

Such a plan has been under theoretical and practical considerations by both industry[3] and academia.[4] However, to the authors' best knowledge, the literature on retrofitting an existing petroleum infrastructure for biorefinery is still quite limited since not many countries have extensive petroleum infrastructure and the urgent to produce biofuel. Mahmoud et al.[5] proposed a study of converting biomass into gasoline and diesel by using the existing refinery to upgrade the biomass intermediates. In one alternative, the biorefinery, and the petroleum refinery are considered stand-alone parallel structures. The other alternative is to integrate the biorefinery network into the petroleum refinery by co-processing the biomass and crudes in the same fluid catalytic cracking unit and hydrocracking unit. Tong et al.[6] considered a hydrocarbon biofuel supply chain integrated with the petroleum refinery. Several integration strategies to insert the bio-oil and bio-slurry with crude stream were analyzed under uncertainty. The drop-in fuels, such as gasoline, diesel, and jet fuel were finally produced. Fuzzy programming was used to address the uncertainty. The same authors extended the work by taking into account the optimal operations to improve the economic performance of such an integrated supply chain under price and demand uncertainties through stochastic programming[7] and robust optimization[8], respectively. Ali et al.[9] conducted a techno-economic evaluation of the co-processing between raw bio-oil and long residue from a fluid catalytic cracking (FCC) unit. Sensitivity analysis was assessed to reveal the economic impact of the selling price on the net present value. Tanzil et al.[10] conducted detailed techno-economic analyses of six sustainable aviation fuel production technologies to obtain a simplified cost estimation method under pre-defined incorporation in a refinery. Based on that, the same authors[11] investigated a typical petroleum refinery under three possible integration scenarios, including sharing infrastructure, co-processing biomass intermediates, and repurposing an idle plant. Lee et al.[12] implemented the life cycle analysis to evaluate the carbon emissions of ci-processing between both pyrolysis oil and the feedstock to an FCC unit. Yazdanparast et al[13] proposed a practical optimization model to consider the potential supply and production disruptions with existing petroleum infrastructure. A risk-averse two-stage stochastic program is developed under different strategies to cope with uncertainty. The authors managed to ensure both economic and environmental sustainability by integrating the planning and operational decisions. Börjesson et al[14] accessed the opportunities to produce sustainable aviation fuel based on existing industrial infrastructures in Sweden. The authors concluded that upgrading the bio-intermediates in the petroleum refinery could reduce the total cost and emissions, leading to commercial development.

From the above literature review, it is quite apparent that the analysis of retrofitting or repurposing existing facilities into a biorefinery is usually conducted with techno-economic analysis under a given fixed flowsheet. The integration or co-processing is predefined in advance so that the economic impact can be determined. While this may leave out the optimal options due to the predefined superstructure. In addition to that, it is also quite rare to consider the production planning along with the retrofitting scheme over a long specified time horizon. In such a case, the problem can be viewed as a multistage problem where the production demand needs to be satisfied in each stage with potential technologies.

Making optimal decisions under uncertainty in such a multistage problem is another major challenge. Stochastic programming (SP) is one of the most widely used techniques to address uncertainty.[15,16] In SP, not all the decisions need to be determined at the beginning. Usually, the decision maker can take actions in each stage corresponding to the realization of the uncertainty, leading to better performance.[17] The uncertainty can be divided into two types: endogenous uncertainty and exogenous uncertainty. Exogenous uncertainty refers to the parameters whose true values are revealed periodically and independently of decisions determined by the decision maker, for example, the demand and price of products. The other type of uncertainty, endogenous uncertainty, refers to the uncertain parameters in which the realizations are decision-dependent. The endogenous uncertainty can be further categorized into two types. The first type refers to the uncertainty whose underlying probability distribution is influenced by decisions[18]; the other type refers to uncertainty whose realization is influenced by the timing of the decision.[19] The modeling of endogenous uncertainty is a recent research area with the first publication in 1998.[20] This area was systematically studied with the gas-field development problem.[19,21] The uncertainty was assumed to be resolved immediately after the decision was made, which was further incorporated in the synthesis of process networks.[22] Major progress was made by Gupta and Grossmann[23,24] by exploiting general theoretical properties to reduce the model dimensions and developing a Lagrangean decomposition algorithm to solve the corresponding large-scale problem effectively. Research on optimization under both endogenous and exogenous uncertainties was conducted by Apap et al.[25] In that work, the endogenous uncertainty is focused on the second type. Regarding the retrofitting optimization problem, although there are several paper[6–8] addressing the uncertainty, the consideration of both endogenous and exogenous uncertainty in this problem is rarely taken into account.

In this paper, a retrofitting optimization problem from a conventional crude-based refinery into a biomass-based biorefinery with given technologies is addressed. The background of the refinery and potential biomass-based technologies are presented in Section 2. The problem is described in Section 3. The mathematical formulations for both the deterministic model and multistage stochastic programming (MSSP) model are described in Section 4. The Lagrangean decomposition algorithm is briefly introduced in Section 5. The discussion of the results of the retrofitting scheme and the computational statistics from MSSP are presented in Section 6. Finally, the conclusions are drawn in Section 7.

2 | BACKGROUND

2.1 | Crude-based Refinery Illustration

A conventional refinery utilizes crude oil to produce desired products, such as gasoline, jet fuel, and diesel. A typical crude-based refinery with a crude distillation capacity of 42,000 kbbl per year is adapted from Zhang et al.[26] and shown in Fig. 1, where the hydrocarbons are identified and marked for each stream in the refinery. The raw crude oil is first distilled in a crude distillation unit (CDU) into liquified petroleum gas (LPG, composed of hydrocarbons C3 to C5), naphtha (NAP, composed of hydrocarbons C5 to C10), kerosene (KERO, composed of hydrocarbons C10 to C16), diesel (DI, composed of hydrocarbons C16 to C22), light gas oil (LGO, composed of hydrocarbons C22 to C40), and residue oil (RESID, composed of hydrocarbons C22+). it is also possible to blend the streams as final products if necessary, such as the KERO, blended in the jet fuel tanks. However, these streams are usually hydrotreated to improve their quality by removing sulfur and nitrogen before being sold as final products. The upgraded hydrocarbons are later cracked or reformed in the following units to obtain high-quality products. For example, the outlet stream from the naphtha hydrotreating unit (NHT), goes through isomerization reactions in the isomerization unit (ISO) to improve the octane number property, which is specified for product gasoline (GASO). Other hydrotreated streams, from the diesel hydrotreating unit (DHT), gas oil hydrotreating unit (GOHT), and residue hydrotreating unit (RDHT), are upgraded in the continuous reforming unit (CCR), fluid catalytic cracking unit (FCC), and hydrocracking unit (HC). Along with the delayed coking unit (DC), the intermediates from these units are blended as the final products, LPG, GASO, jet fuel (JET), diesel (DIESEL), and fuel oil (OIL) under corresponding quality specifications, such as specific gravity (SG), research octane number (RON). However, due to the inherent nonlinearity, the property of mixed streams is often determined by highly nonlinear relations. To avoid that, the property index[27] can be used to replace the property so that the mixture of crudes can be modeled to be linear. The conversions of property to respective property index can be found in Appendix.

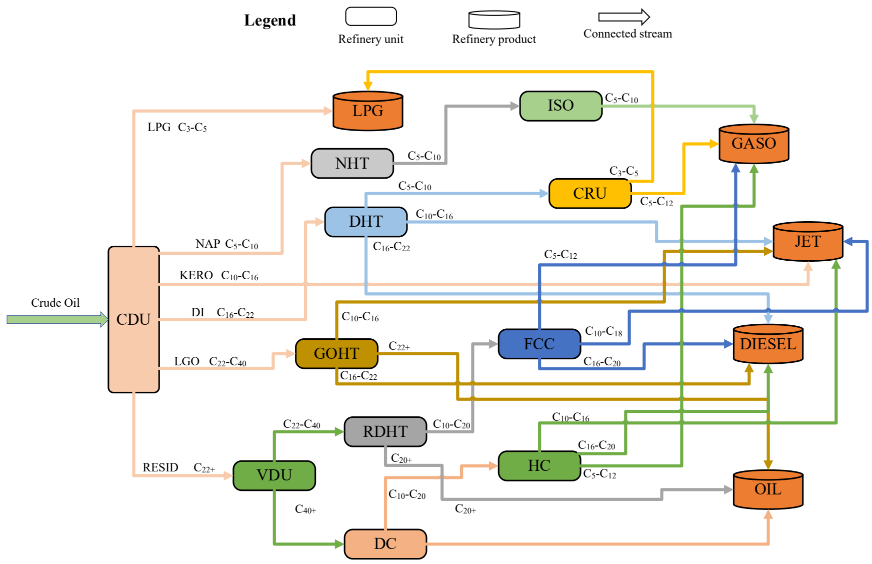


Fig. 1 Flowsheet of a given crude-based refinery.

The potential connections between streams and operation units are presented in Table. 1. In retrofitting optimization, it is apparent that one or more refinery units would be used to process the biomass streams in the selected biomass-based technologies so that the related flows need to be redirected to other operating units to meet the crude demands. By comparing the detailed components of the inlet streams and outlet streams in each refinery unit, the underlying redirections between crude streams and refinery units can be determined in advance. For example, the DC unit can process the hydrocarbons of C22+ via coking reactions and produce two intermediate hydrocarbon products, C9 – C20 and C20+. The lighter stream can be fed into the FCC or HC unit since these units usually process crudes that have similar hydrocarbons. If the FCC is used in biomass-based technologies, this flow can be processed in the HC unit alternatively. By recognizing potential connections, the pathways in the conventional refinery can be maintained to provide crude products.

Table.1 Potential retrofitting between crude-based refinery units.

Feedstock	Operation unit	Outlet intermediates	Possible redirected units/products
Crude oil	CDU	LPG (C3 – C5)	LPG
		NAP (C5 – C10)	NHT/GASO
		KERO (C10 – C16)	DHT/DIESEL
		DI (C16 – C22)	DHT/DIESEL
		LGO (C22 – C40)	GOHT/RDHT
		RESID (C22 – C40)	VDU
C22+	VDU	VGO (C22-C40)	GOHT/RDHT
		HGO (C40+)	DC/OIL
C5 – C10	NHT	C5 – C10	CRU/ISO/GASO
C10 – C22	DHT	C5 – C10	CRU/ISO/GASO
		C10 – C16	FCC/HC/JET
		C16 – C22	FCC/HC/DIESEL
C18 – C40	GOHT	C10 – C16	FCC/HC/JET
		C16 – C22	FCC/HC/DIESEL
		C22+	OIL
C22 – C40	RDHT	C10 – C20	FCC/HC/JET
		C22+	DC/OIL
C22+	DC	C9 – C20	FCC/HC
		C20+	OIL
C5 – C10	ISO	C5 – C10	CRU/GASO
C5 – C12	CRU	C3 – C5	LPG
		C5 – C12	GASO
C9 – C20	FCC	C5 – C10	GASO
		C10 – C16	JET
		C16 – C22	DIESEL
C9 – C20	HC	C5 – C10	GASO
		C10 – C16	JET
		C16 – C22	DIESEL

2.2 | Biomass-based Technology Illustration

In this work, six biomass-based technologies that process biomass into hydrocarbons, are selected as potential alternatives. Namely, hydroprocessed esters and fatty acids (HEFA), Virent's BioForming (VB), alcohol to jet (ATJ), direct sugar to hydrocarbon (DSHC), fast pyrolysis (FP), and gasification and Fischer-Tropsch (GFT). The main steps and material flow for these alternatives are presented in Fig. 2. It should be mentioned that in each figure, the coloured stages represent the operation that can be executed in the respective refinery units. And the final distillation operations can be done in the refinery CDU to separate the bio-products.

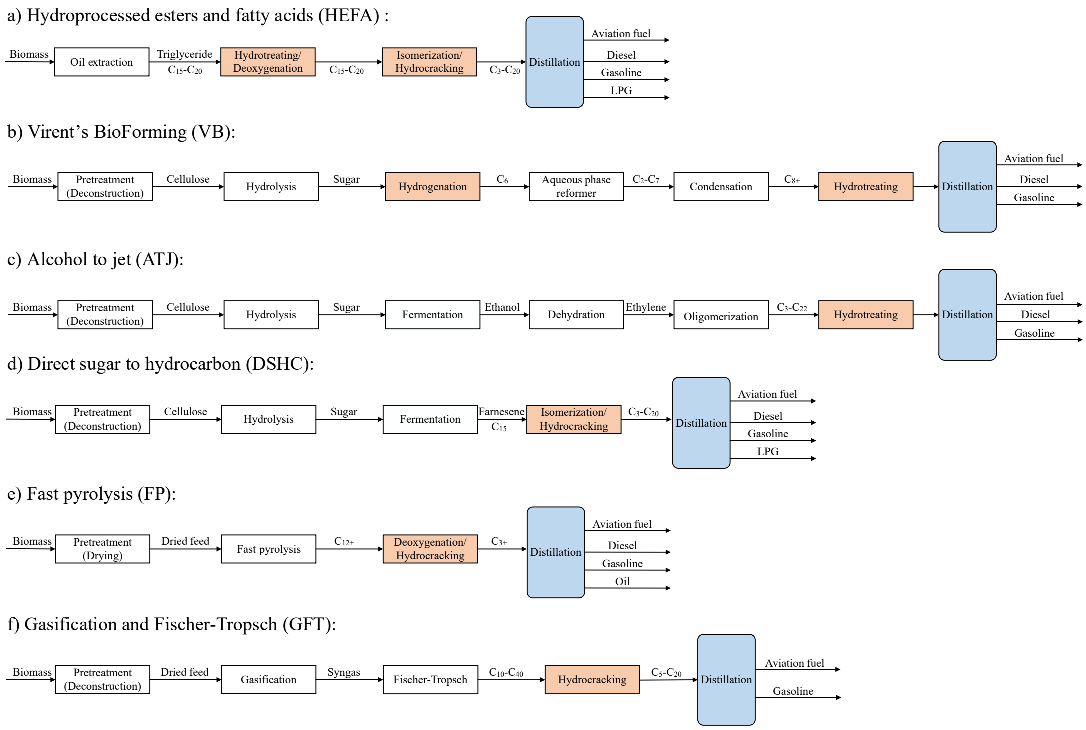


Fig. 2. Main steps and material flow in biomass-based technologies.

HEFA has been approved by the American Society for Testing and Materials[28] as a possible pathway whose products can be blended up to 50% with petroleum-based jet fuel for sustainable aviation fuel. This technology processes the biomass that contains triglycerides, such as animal fats[29], and vegetable oil[30], into hydrocarbons through a series of stages[31]. First, the triglyceride is obtained from the biomass through oil extraction. The intermediate is then hydrotreated in the respective unit where the oxygen is also removed. Following, the linear paraffinic hydrocarbon is isomerized to improve the property of the fuel. Along with isomerization, the hydrocracking reaction also occurs in such unit, and lighter hydrocarbon is obtained. The stream is separated into final products, LPG, diesel, gasoline, and aviation fuel through distillation. In this technology, as marked in Fig. 2(a), the hydrotreating and isomerization steps can be processed in the refinery hydrotreating units and isomerization units, respectively.

The VB technology is designed to upgrade the feedstock (usually lignocellulose and starch) via a catalytic process, as shown in Fig. 2(b).[32] The purified cellulose stream, from the deconstructed biomass, undergoes the hydrolysis reaction and converts it into sugar under the catalytic effect of cellulase enzymes. The sugar is then hydrogenated and undergoes aqueous phase reforming (APR), which converts the sugar alcohols into light alkanes. The light hydrocarbons are turned into long-chain hydrocarbons within the condensation step.[33] Same as the HEFA technology, the final hydrotreating process removes leftover oxygen, and finally, the stream is separated into aviation fuel, diesel, and gasoline. Within such steps, the hydrotreating processes can be operated in the refinery hydrotreating units.

In addition to the VB technology, the ATJ technology also utilizes sugars to produce aviation fuel.[34] The schematic biochemical pathway for ATJ is illustrated in Fig 2(c). Similar to the VB technology, the raw material is first converted into sugar under deconstruction and hydrolysis, followed by the fermentation step to produce ethanol. Next, the ethanol is dehydrated and converted into ethylene, which is processed through oligomerization and hydrotreating sequentially.[35] The olefins from dehydration are converted into long-chain hydrocarbons by oligomerization reaction. After the final hydrogenation step, the final products are obtained. In ATJ, the hydrotreating step is the only process that can be executed in a certain hydrotreating unit.

Another alternative similar to VB and ATJ is the DSHC technology, which converts the sugar into farnesene. The biomass feedstock, lignocellulose or starch, is used as the source of the sugar stream. The sugar is then fermented to obtain the long-chain hydrocarbons, which are later hydrocracked, isomerized, and distilled into final products.[36,37] Aviation fuel, diesel, gasoline, and LPG can be produced through such biomass pathways. The last step before distillation can be executed in the respective refinery HC or ISO unit due to the similar chemical process.

Thermochemical processes are also considered in this study. The widely studied FP technology, presented in Fig. 2(e), first heats the biomass to between 450 and 550 ℃ so that the production of the liquid pyrolysis oil can be maximized.[38] Followed by the two-step hydrotreatment process, hydrodeoxygenation, and hydrocracking reactions, the oxygenated bio-oil is upgraded to satisfy the quality specification of final products, including aviation fuel, diesel, gasoline, and oil. The deoxygenation step, also regarded as a hydrocracking unit, is assumed to be a step that can be processed in the refinery unit.

The thermochemical process GFT can convert the biomass feedstock into syngas which is a mixture of CO and H_2.[39] After cooling down and removing the contaminants, the syngas is converted into long-chain hydrocarbons in the Fischer-Tropsch process.[40] To obtain the final aviation fuel and gasoline products, the stream is cracked into shorter-chain hydrocarbons, which can be processed in the refinery HC unit. It should be mentioned that, in each technology, the products are separated via a distillation step which can also be processed in the CDU from the crude refinery.

3 | PROBLEM STATEMENT

Given the existing refinery in Fig.1 and six potential technologies as described in Section 2, the goal of this paper is to optimize the retrofit from a conventional crude-based refinery into a biomass-based biorefinery with production planning in specified periods. Specifically, it is assumed that the following is given:

1. Specified time horizon and discrete time period (also treated as a year);
2. Production details for the given six biomass-based technologies, including the yield and property of the intermediates and products;
3. Available crude oil assay data for each year, including the available supply and true boiling point data;
4. Predicted demands and prices of both crude and biomass products for each year;
5. Data of capacity, products yield, processing cost, reconnection, and retrofitting cost for each refinery or biorefinery unit;
6. Quality specification for both crude and biomass products;
7. Conversion relation between specified quality and quality index; (Seen in the Appendix)
8. Under the consideration of demand and yield uncertainty, the probability and uncertainty values in different scenarios are given.

With such assumptions, the objective of this problem is to minimize the total retrofit and production cost while making the following decisions in a deterministic model. Regarding the stochastic programming problem, the objective is to minimize the expected cost over all the possible scenarios.

1. Retrofit scheme to satisfy the fuel requirements each year;
2. Production planning for processing crude and biomass each year;
3. Biomass feedstock to respective refinery units in biomass-based technologies;
4. Final blending decisions of desired crude and biomass products each year;
5. Unit construction and capacity expansion in selected technologies each year.

Next, the MILP formulation for the deterministic model is presented and extended into multistage stochastic programming (MSSP). The data for this problem is adapted from Tanzil et al.[10,11]

3.1 | Deterministic Model

The objective of this ten-year retrofit problem is to minimize total cost by subtracting sales income from the summation of material cost, operation cost, reconnection cost, and construction cost, as shown in Eq. (1).

$$min\ z = cost^{feed} + cost^{equi} + cost^{oper} - income^{sale} \tag{1}$$

$$s.t.\quad cost^{feed} = \sum_{t\in T, c\in C} pr^{cru}_{t,c} F^{in}_{t,c} + \sum_{t\in T, b\in B} pr^{bio}_{t,b} F^{in}_{t,b} \tag{2}$$

$$cost^{equi} = \sum_{k\in K, u\in U^b, l\in L} co^{equi,up}_{k,u,l} \lambda^{up}_{k,u,l} + co^{equi,lo}_{k,u,l} \lambda^{lo}_{k,u,l} + \sum_{k\in K, u\in U^r, u'\in U^b} co^{sub}_{u,k,u'} y^{sub}_{u,k,u'} \tag{3}$$

$$cost^{oper} = \sum_{t\in T, u\in U^r \cup U^b} co^{oper}_{u} F^{in}_{t,u} \tag{4}$$

$$income^{sale} = \sum_{t\in T,p\in P^r} pr_{t,p}^{sale} F_{t,p}^{sale} + \sum_{t\in T,p\in P^b} pr_{t,p}^{sale} F_{t,p}^{sale} \quad (5)$$

The terms appearing in the objective function are explicitly shown in Eqs. (2) – (5). Considering each potential feedstock crude oil $c \in C$ and biomass $b \in B$, the material cost is defined by multiplying the price and processing amount in each year $t \in T$. The equipment cost, including the equipment cost for the new-constructed unit and the reconnection cost of implementing existing refinery units into the selected biomass-based technologies, is given in Eq. (3). These two terms are defined with the binary variables $y_{k,u,l}^{equi}$ and $y_{u,k,u'}^{sub}$ to denote if a unit is constructed or a unit is retrofitted, respectively. For each new-constructed unit, the concave cost function related to the capacity is approximated by the piecewise linearization method for each interval $l \in L$. The cost for the lower capacity and upper capacity within the interval $l \in L$ are given with constants $co_{k,u,l}^{equi,lo}$ and $co_{k,u,l}^{equi,up}$, respectively. The piecewise linearization is defined with nonnegative continuous variables $\lambda_{k,u,l}^{lo}$ and $\lambda_{k,u,l}^{up}$ (where $\lambda_{k,u,l}^{lo}, \lambda_{k,u,l}^{up} \in [0,1]$) which are defined as the linear weight variables for unit u of biomass-based technology k in interval l. The continuous variables $\lambda_{k,u,l}^{lo}$ and $\lambda_{k,u,l}^{up}$ are activated by determining the binary variable $y_{k,u,l}^{quip}$. The cost to implement a refinery unit into a biorefinery unit is denoted by multiplying the binary variable $y_{u,k,u'}^{sub}$ and related cost $co_{u,k,u'}^{sub}$ with refinery unit $u \in U^r$ and biorefinery unit $u \in U^b$. For each processing unit, the operation cost is defined by multiplying a constant parameter and the total flowrate of the respective feedstock $F_{t,u}^{in}$. In each year, the products are sold according to the demand, and the sale income is defined as the summation product of price and sale amount regarding refinery products $p \in P^r$ and biomass products $p \in P^b$ as shown in Eq. (5). Note that the cost minimization in Eq. (1) is equivalent to maximizing the negative value of the net profit. For convenience, the minimization objective function is kept which treats the profit as a negative cost.

Eqs. (6) – (17) describe the explicit constraints for the crude refinery units. The CDU is modeled via the swing-cut technique[41] with given data for each crude oil. The binary variable $y_{t,c}^{cru}$ denotes a specific type c of crude that is selected in year t if $y_{t,c}^{cru}$ equals to 1, and the related flowrate constraints derived from inventory and capacity are defined in Eq. (6) and Eq. (7), respectively. The mass balance between feedstock and intermediates or products is given by Eqs. (8) – (10) with the swing-cut stream $w \in W$ dispatching to adjacent intermediates. The yield parameters are assumed to be constants for the different crudes. The intermediates from CDU are delivered to the following units and products in the refinery, shown in Eq. (11). Similarly, Eqs. (12) – (14) define the mass balance for each unit. In Eq. (15), the decision on whether to implement operation unit u' in biomass-based technology k with refinery unit u is denoted by binary variables $y_{t,u,k,u'}^{nonco}$ and $y_{t,u,k,u'}^{co}$. If $y_{t,u,k,u'}^{co}$ equals to 1, the unit can process both biomass stream and crude stream in the same year, while if $y_{t,u,k,u'}^{nonco}$ equals to 1 the unit can only process bio-materials in year t. The logic of these operations is defined with a new binary variable $Y_{t,u}^{nonco}$ and disjunctions defined in Eqs. (16) – (17).

$$y_{t,c}^{cru} Inv_{t,c}^{lo} \le F_{t,c}^{in} \le y_{t,c}^{cru} Inv_{t,c}^{up} \quad \forall c \in C, t \in T \tag{6}$$

$$y_{t,c}^{cru} Cap_{CDU}^{lo} \le F_{t,c}^{in} \le y_{t,c}^{cru} Cap_{CDU}^{up} \quad \forall c \in C, t \in T \tag{7}$$

$$F_{t,c,w} = F_{t,c}^{in} Yield_{c,w} \quad \forall t \in T, c \in C, w \in W \tag{8}$$

$$F_{t,c,w} = \sum_{s \in S^c} F_{t,c,w,s} \quad \forall t \in T, c \in C, w \in W \tag{9}$$

$$F_{t,c,s}^{out} = F_{t,c}^{in} Yield_{c,s} + \sum_{w \in W} F_{t,c,w,s} \quad \forall t \in T, c \in C, s \in S^c \tag{10}$$

$$F_{t,c,s}^{out} = \sum_{u \in U^r} F_{t,c,s,u} + \sum_{p \in P^r} F_{t,c,s,p} \quad \forall t \in T, c \in C, s \in S^c \tag{11}$$

$$F_{t,u}^{in} = \sum_{c \in C, s \in S^c} F_{t,c,s,u} + \sum_{u' \in U^r, s \in S} F_{t,u',s,u} \quad \forall t \in T, u \in U^r \tag{12}$$

$$F_{t,u,s}^{out} = F_{t,u}^{in} Yield_{u,s} \quad t \in T, u \in U^r, s \in S \tag{13}$$

$$F_{t,u,s}^{out} = \sum_{p \in P^r} F_{t,u,s,p} + \sum_{u' \in U^r} F_{t,u,s,u'} \quad t \in T, u \in U^r, s \in S \tag{14}$$

$$\sum_{k \in K, u' \in U^b} (y_{t,u,k,u'}^{nonco} + y_{t,u,k,u'}^{co}) \le 1 \quad \forall t \in T, u \in U^r \tag{15}$$

$$Y_{t,u}^{nonco} \Leftrightarrow \bigvee_{k \in K, u' \in U^b} y_{t,u,k,u'}^{nonco} \quad \forall t \in T, u \in U^r \tag{16}$$

$$\begin{bmatrix} Y_{t,u}^{nonco} \\ F_{t,u}^{in} = 0 \end{bmatrix} \vee \begin{bmatrix} \neg Y_{t,u}^{nonco} \\ Cap_u^{lo} \le F_{t,u}^{in} \le Cap_u^{up} \end{bmatrix} \quad \forall t \in T, u \in U^r \tag{17}$$

Regarding the selection of biomass-based technology and retrofitting decisions, Eqs. (18) – (31) define the explicit constraints for capacity expansion and production planning in the biorefinery. Binary variable $y_{t,k}^{op}$ is used to denote whether a technology k is operated in year t, and feedstock selection is represented by the binary variable $y_{t,k,b}^{feed}$ for technology k. Eq. (18) denotes that if the technology k is operating at year t, at most one biomass feedstock can be selected. Furthermore, the flowrate of processed biomass is constrained by Eq. (19) with its available inventory. For the units to be constructed, the capacity of unit u in technology k at year t is defined with continuous variable $ca_{t,k,u}$ and the expanded capacity in each year is represented by $ca^{exp}_{t,k,u}$ so that the relation of capacity between years can be represented via Eqs. (20) – (22). The mass balance equalities are defined with Eqs. (23) – (26) where u^{b}_{pre} denotes the pre-treatment step and u^{b}_{dis} denotes the distillation step, which is usually the final step in each technology. It should be mentioned that the yield for each stream is assumed to be constant, denoted by the parameter $Yield_{k,b,u,s}$. To model the mass balance constraints of retrofit, the feedstock of each step is divided into two parts, $F^{sub}_{t,k,u,u'}$ and $F^{new}_{t,k,u}$ in Eq. (27). The continuous variable $F^{sub}_{t,k,u,u'}$ represents the flowrate from bio-unit u to refinery unit u', which is constrained with related retrofitting decisions, shown in Eqs. (28) – (30). The variable $F^{new}_{t,k,u}$ defines the flowrate, which is processed in the newly constructed unit and constrained in Eq. (31).

$$\sum_{b} y^{feed}_{t,k,b} = y^{op}_{t,k} \quad \forall t \in T, k \in K \tag{18}$$

$$y^{feed}_{t,k,b} Inv^{lo}_{t,b} \leq F^{in}_{t,k,b} \leq y^{feed}_{t,k,b} Inv^{up}_{t,b} \quad \forall t \in T, k \in K, b \in B \tag{19}$$

$$ca_{t,k,u} = ca_{t-1,k,u} + ca^{exp}_{t,k,u} \quad \forall t \in T, k \in K, u \in U^{b} \tag{20}$$

$$Cap^{lo}_{t,k,u} y^{exp}_{t,k,u} \leq ca^{exp}_{t,k,u} \leq Cap^{up}_{t,k,u} y^{exp}_{t,k,u} \quad \forall t \in T, k \in K, u \in U^{b} \tag{21}$$

$$\sum_{k \in K, u \in U^{b}} ca^{exp}_{t,k,u} \leq Cap^{exp,up}_{t} \quad \forall t \in T \tag{22}$$

$$F^{in}_{t,k,b} = F^{in}_{t,k,b,u} \quad \forall t \in T, k \in K, b \in B, u \in \{u^{b}_{pre}\} \tag{23}$$

$$F^{out}_{t,k,b,u,s} = F^{in}_{t,k,b,u} Yield_{k,b,u,s} \quad \forall t \in T, k \in K, b \in B, u \in U^{b}, s \in S^{b} \tag{24}$$

$$F^{in}_{t,k,b,u} = F^{out}_{t,k,b,s,u-1} \quad \forall t \in T, k \in K, b \in B, u \in U^{b} \backslash \{u^{b}_{pre}\}, s \in S^{b} \tag{25}$$

$$F^{out}_{t,k,b,u,s} = \sum_{p \in P^{b}} F_{t,k,b,u,s,p} \quad \forall t \in T, k \in K, b \in B, u \in \{u^{b}_{dis}\}, s \in S^{b} \tag{26}$$

$$\sum_{b} F^{in}_{t,k,b,u} = \sum_{u' \in U^{r}} F^{sub}_{t,k,u,u'} + F^{new}_{t,k,u} \quad \forall t \in T, k \in K, u \in U^{b} \tag{27}$$

$$F^{sub}_{t,k,u,u'} \leq \left(y^{nonco}_{t,u',k,u} + y^{co}_{t,u',k,u}\right) Cap^{up}_{u'} \quad \forall t \in T, k \in K, u \in U^{b}, u' \in U^{r} \tag{28}$$

$$Y^{co}_{t,u} \Leftrightarrow \bigvee_{k \in K, u' \in U^{b}} y^{co}_{t,u,k,u'} \quad \forall t \in T, u \in U^{r} \tag{29}$$

$$\left[\begin{array}{c} Y^{co}_{t,u} \\ Cap^{lo}_{u} \leq F^{in}_{t,u} + \sum_{k \in K, u' \in U^{b}} F^{sub}_{t,k,u',u} \leq Cap^{up}_{u} \end{array}\right] \quad \forall t \in T, u \in U^{r} \tag{30}$$

$$\alpha_{k,u}^{min} ca_{t,k,u} \leq F_{t,k,u}^{new} \leq \alpha_{k,u}^{max} ca_{t,k,u} \quad t \in T, k \in K, u \in U^b \tag{31}$$

Constraints on final products and construction costs are given in Eqs. (32) – (38). The crude products are denoted with $p \in P^r$, while the biorefinery products are defined as $p \in P^b$. The mass balance, as well as the quality specification of products, are specified in Eqs. (32) – (35). Here the property is assumed to be known as constants for each stream and converted into a property index in Eqs. (33) and (35). The sale of the final products should be within the estimated demand, as shown in Eq. (36). Binary variable $y_{u,k,u'}^{sub}$ is used to denote if a refinery unit u is implemented as a bio-unit ever once in Eq. (37). As for the equipment expense appearing in Eq. (3), the piecewise linearization of the concave cost function for bio-units is defined in Eqs. (38) – (40). The binary variable $y_{k,u,l}^{quip}$ is defined to represent the piecewise capacity assignment related to the final capacity of the new-built unit. The values of continuous variables λ can be determined with constraint $\lambda_{k,u,l}^{lo} + \lambda_{k,u,l}^{up} = 1$ or $\lambda_{k,u,l}^{lo} + \lambda_{k,u,l}^{up} = 0$ for unit u of biomass-based technology k, related to the values of final capacity $ca_{t^e,k,u}$ and binary variable $y_{k,u,l}^{quip}$ for each interval l.

$$F_{t,p}^{sale} = \sum_{u \in U^r, s \in S} F_{t,u,s,p} + \sum_{c \in C, s \in S^c} F_{t,c,s,p} \quad \forall t \in T, p \in P^r \tag{32}$$

$$F_{t,p}^{sale} E_p^{lo} \leq \sum_{u \in U^r, s \in S} F_{t,u,s,p} E_{u,s} + \sum_{c \in C, s \in S^c} F_{t,c,s,p} E_{c,s} \leq F_{t,p}^{sale} E_p^{up} \quad \forall t \in T, p \in P^r \tag{33}$$

$$F_{t,p}^{sale} = \sum_{k \in K, b \in B, s \in S} F_{t,k,b,u,s,p} \quad \forall t \in T, p \in P^b, u \in \{u_{dis}^b\} \tag{34}$$

$$F_{t,p}^{sale} E_p^{lo} \leq F_{t,k,b,u,s,p} E_{k,b,u,s} \leq F_{t,p}^{sale} E_p^{up} \quad \forall t \in T, p \in P^b \tag{35}$$

$$demand_{t,p}^{lo} \leq F_{t,p}^{sale} \leq demand_{t,p}^{up} \quad \forall t \in T, p \in P^r \cup P^b \tag{36}$$

$$y_{t,u,k,u'}^{nonco} + y_{t,u,k,u'}^{co} \leq y_{u,k,u'}^{sub} \quad \forall t \in T, u \in U^r, k \in K, u' \in U^b \tag{37}$$

$$y_{k,u,l}^{quip} Capl_l^{up} \leq ca_{t^e,k,u} \leq y_{k,u,l}^{quip} Capl_l^{up} \quad \forall k \in K, u \in U^b, l \in L \tag{38}$$

$$ca_{t^e,k,u} = \lambda_{k,u,l}^{lo} Capl_l^{lo} + \lambda_{k,u,l}^{up} Capl_l^{up} \quad \forall k \in K, u \in U^b, l \in L \tag{39}$$

$$\lambda_{k,u,l}^{lo} + \lambda_{k,u,l}^{up} = y_{k,u,l}^{quip} \quad \forall k \in K, u \in U^b, l \in L \tag{40}$$

3.2 | Multistage Stochastic Programming Model

The deterministic model is then extended to Multistage Stochastic Programming (MSSP) model by taking into account the endogenous yield uncertainty and exogenous demand uncertainty. The MSSP formulation can be obtained via duplicating variables into scenarios and adding extra non-anticipativity constraints (NACs) as shown in Fig.

3. The NACs are represented by the dashed lines which connect two linked scenarios. In such two scenarios, the decision variables should be equal since the revealed uncertainties are the same up to the current stage. By applying such a mathematical formulation, the size of the proposed model increases exponentially with the total scenarios and stages, leading to very large computational expenses.

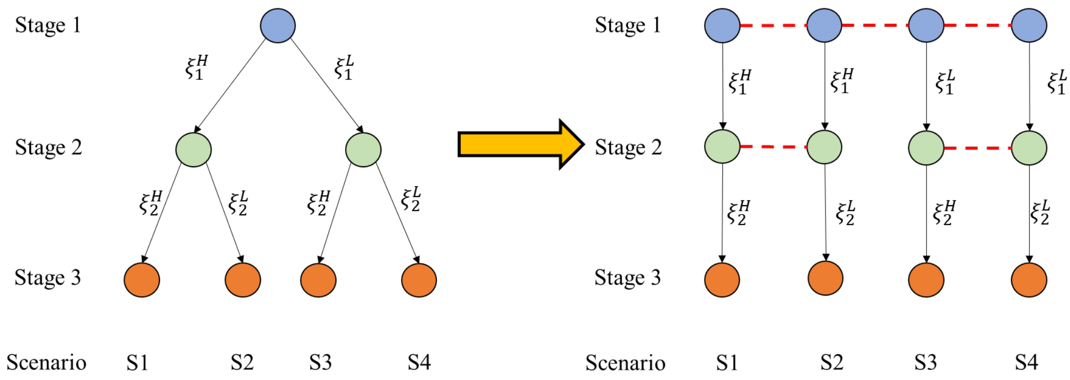


Fig. 3. Demonstration of alternative scenario tree.

In this retrofit optimization problem, each year is considered a stage. Regarding the endogenous yield uncertainty, each biomass-based technology is assumed to have two possible values, high and low, leading to 64 scenarios in total. Only the demands for three bio-products, green gasoline, green diesel, and sustainable aviation fuel, are assumed to be uncertain. For the exogenous uncertainty, three levels, low, medium, and high demands are used for these products every year, leading to a total of 27^{10} scenarios. Combining both endogenous and exogenous uncertainty, there are 64×27^{10} scenarios, causing a curse of dimensionality. To reduce the number of scenarios and make the problem more manageable, the MSSP is formulated with the following strategy.[42] The decisions are first divided into strategic decisions and operational decisions. The strategic decisions are defined as the critical decisions that are made once for the expansion of the biorefinery, including the selection of biomass-based technology, capacity expansion, and unit substitution. These decisions usually affect long-term operations and are assumed to be related to endogenous uncertainty. The operational decisions are defined as the decisions made each year to satisfy the product requirements and material supply, such as the type of crude oil, and sale decisions for products. These operational decisions are assumed to be related to demand uncertainty since the decisions are determined under the realizations of demand. The exogenous demand uncertainty is also assumed to be independent each year, which means the demand uncertainty in stage t is not affected by the uncertainty in other stages.

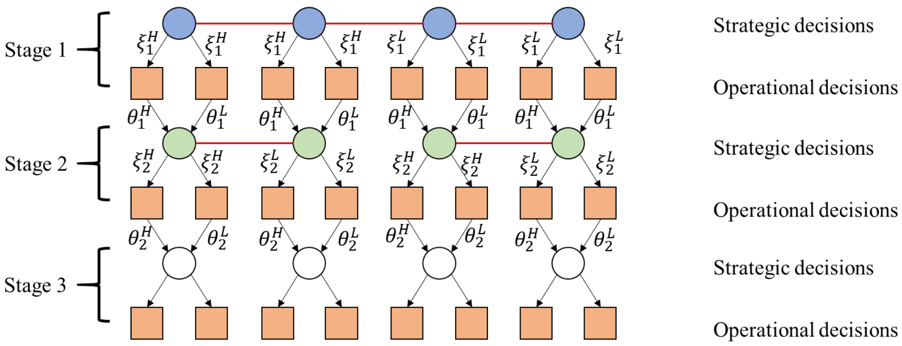


Fig. 4. Proposed formulation of the scenario tree.

Given the above assumptions, the MSSP problem is then formulated as follows.[25] The set $i \in I$ denotes the scenarios corresponding to endogenous yield uncertainty and set $j \in J$ denotes the scenarios related to exogenous demand uncertainty appearing each year. Each year, the problem can be viewed as a two-stage stochastic programming subproblem. At the beginning of the year, strategic decisions need to be determined. The demand uncertainty is then realized and the operational decisions are made to satisfy the requirement for products. In such a modeling framework, the set $i \in I$ is considered as the main scenario to divide the full-space model into subproblems and the strategic decision is rather important to ensure that the retrofitted biorefinery should be able to satisfy all the possible demands for the products. The set $j \in J$, which is related to demand uncertainty and appears each year, is incorporated in each stage. The general mathematical formulation can then be written as follows:

$$min\ z = \sum_{i \in I} p_i \left(\sum_{t \in T} c_{t,i} y_{t,i} + \sum_{t \in T, j \in J} p_{t,j} d_{t,i,j} x_{t,i,j}\right) \qquad \text{MSSP-(1)}$$

$$s.t. \quad \sum_{\tau \le t} a_{\tau,i} y_{\tau,i} + n_{\tau,i} x_{\tau,i} \le b_{t,i} \quad \forall t \in T, i \in I \qquad \text{MSSP-(2)}$$

$$e_{t,i} y_{t,i} + f_{t,i,j} x_{t,i,j} \le g_{t,i,j} \quad \forall t \in T, i \in I, j \in J \qquad \text{MSSP-(3)}$$

$$y_{t,i} = y_{t,i'} \quad \forall t \in \{T_1\}, i, i' \in I \qquad \text{MSSP-(4)}$$

$$x_{t,i} = x_{t,i'} \quad \forall t \in \{T_1\}, i, i' \in I \qquad \text{MSSP-(5)}$$

$$Z_{t,i,i'} \Leftrightarrow F(y_{t1,i}, y_{t2,i} \dots y_{t-1,i}) \quad \forall t \in T \backslash \{T_1\}, i, i' \in I \qquad \text{MSSP-(6)}$$

$$\begin{bmatrix} Z_{t,i,i'} \\ y_{t,i} = y_{t,i'} \\ x_{t,i} = x_{t,i'} \end{bmatrix} \vee \left[\neg Z_{t,i,i'}\right] \quad \forall t \in T \backslash \{T_1\}, i, i' \in I \qquad \text{MSSP-(7)}$$

$$y_{t,i} \in \{0,1\} \quad \forall t \in T, i \in I \qquad \text{MSSP-(8)}$$

$$x_{t,i}, x_{t,i,j} \in R \quad \forall t \in T, i \in I, j \in J \qquad \text{MSSP-(9)}$$

The parameter p_i denotes the probability of scenario i, and the parameter $p_{t,j}$ represents the probability for the scenario j which appears in year t. The constraints MSSP-(4) and MSSP-(5) denote the non-anticipativity constraints (NACs) in the first year when no information about the uncertainty is revealed. The binary variable $Z_{t,i,i'}$ is defined to represent whether the two scenarios i and i' are equal or not. The logical constraints on the binary variable are presented in MSSP-(6) where the two scenarios are treated as different scenarios when the true value of the key uncertain parameter is realized. If $Z_{t,i,i'}$ is true, then the strategic decision for both scenarios i and i' should be equal at the year t as specified in constraint MSSP-(7).

4 | LAGRANGEAN DECOMPOSITION ALGORITHM

To solve the MSSP problem, the Lagrangean decomposition algorithm is implemented to address the complicating NAC constraints. The main idea of the algorithm is to decompose the full space model into scenario pairs and then solve the subproblems sequentially by the scenario pairs. To reduce the total number of scenario pairs and subproblems, several model reduction theorems are applied from the Gupta et al.[23] The main steps of the algorithm are shown in Fig. 5.

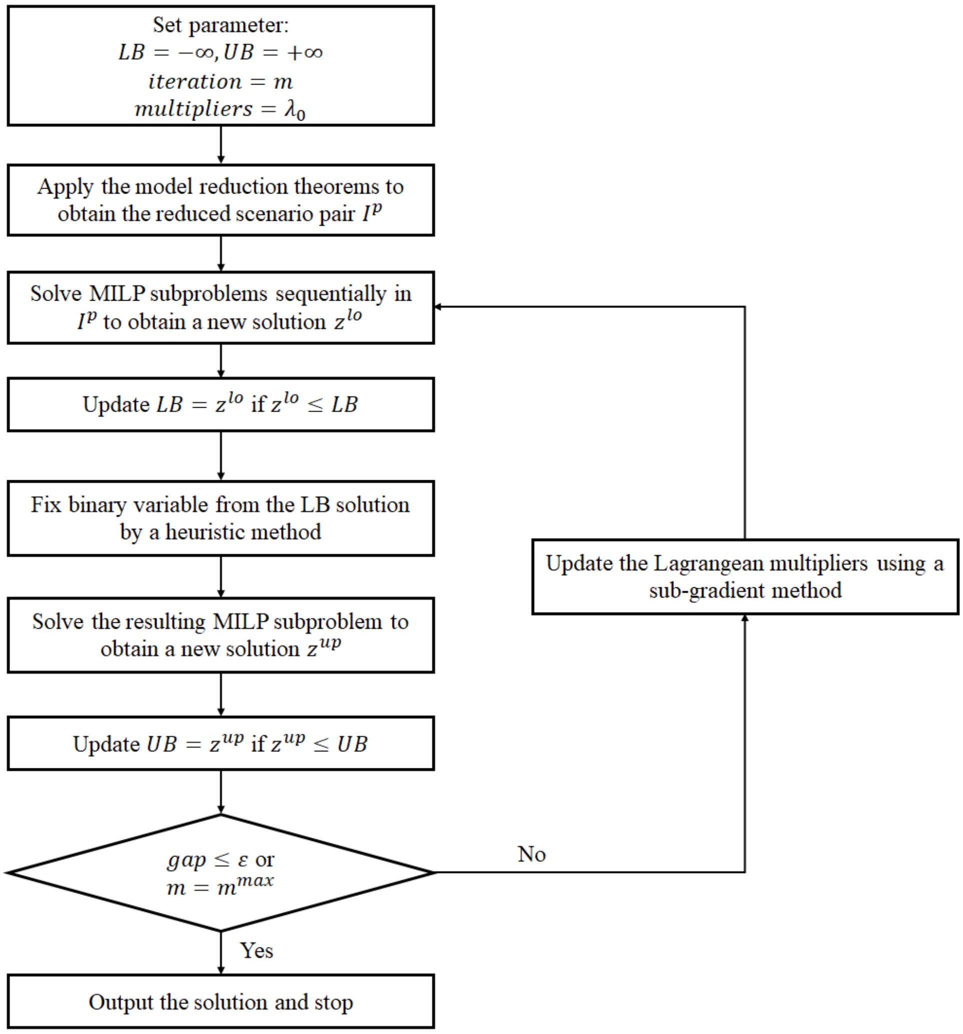


Fig. 5. Lagrangean decomposition algorithm framework.

With the given fixed multipliers, the first time-period NACs are dualized in the objective while other NACs are left out. Therefore, the full space model is decomposed into scenario pairs I^p, whose mathematical formulation can be written as follows:

$$\min z_{I_c^p} = \sum_{i \in I_c^p} p_i \left(\sum_{t \in T} c_{t,i} y_{t,i} + \sum_{t \in T, j \in J} p_{t,j} d_{t,i,j} x_{t,i,j} \right)$$

$$+ \sum_{(i,i') \in I^p} \sum_{t \in \{T_1\}} \lambda_{i,i'} y_{t,i} + \sum_{(i,i') \in I^p} \sum_{t \in \{T_1\}} \lambda_{i,i'} x_{t,i}$$

$$- \sum_{(i',i) \in I^p} \sum_{t \in \{T_1\}} \lambda_{i',i} y_{t,i} - \sum_{(i',i) \in I^p} \sum_{t \in \{T_1\}} \lambda_{i',i} x_{t,i}$$

$$s.t. \quad \sum_{\tau \le t} a_{\tau,i} y_{\tau,i} + n_{\tau,i} x_{\tau,i} \le b_{t,i} \quad \forall t \in T, i \in I_c^p \qquad LD^{I^p}$$

$$e_{t,i} y_{t,i} + f_{t,i,j} x_{t,i,j} \le g_{t,i,j} \quad \forall t \in T, i \in I, j \in J$$

$$Z_{t,i,i'} \Leftrightarrow F(y_{t1,i}, y_{t2,i} \dots y_{t-1,i}) \quad \forall t \in T \backslash \{T_1\}, i, i' \in I_c^p$$

$$\begin{bmatrix} Z_{t,i,i'} \\ y_{t,i} = y_{t,i'} \\ x_{t,i} = x_{t,i'} \end{bmatrix} \vee [\neg Z_{t,i,i'}] \quad \forall t \in T \backslash \{T_1\}, i, i' \in I_c^p$$

$$y_{t,i} \in \{0,1\} \ \forall t \in T, i \in I_c^p$$

$$x_{t,i}, x_{t,i,j} \in R \quad \forall t \in T, i \in I_c^p, j \in J$$

Here, the set I_c^p denotes the scenario pair for the corresponding subproblems and the set I^p denotes the total scenario pairs after reduction. After solving the subproblems in one iteration, a lower bound (LB) can be obtained by adding the optimal objectives of all the subproblems. The upper bound (UB) is then obtained by solving the MILP subproblem derived from fixing binary variables from the LB solution. However, it should be mentioned that the binary variables may lead to a conflict since the NACs are ignored. This can cause infeasibility in the resulting MILP model. Thus, a heuristic rule is used here to determine the binary variables only if there are conflicts between the scenarios. In other words, the binary variables are validated and fixed to the values stage by stage to ensure the NACs can be satisfied. Then the full-space model can be reduced and becomes easier to solve. Solving such a reduced problem provides a feasible solution which is regarded as the UB in this iteration. The algorithm is stopped if the criteria are satisfied (tolerance or maximum iterations). Otherwise, the sub-gradient method is implemented to update the Lagrangean multipliers with the current solution.[43] To be explicit, the procedure can be formulated as follows:

$$\lambda_{i,i'}^{m+1} = \lambda_{i,i'}^{m} + \frac{\theta_{i,i'}^{m} (UB - z^{m,lo}) (y_{T1,i} - y_{T1,i'})}{\left\| y_{T1,i} - y_{T1,i'} \right\|^2} \quad \forall (i',i) \in I^p \qquad (41)$$

$$\lambda_{i,i'}^{m+1} = \lambda_{i,i'}^{m} + \frac{\theta_{i,i'}^{m}(UB - z^{m,lo})\left(x_{T1,i} - x_{T1,i'}\right)}{\left|\left|x_{T1,i} - x_{T1,i'}\right|\right|^2} \quad \forall (i', i) \in I^p \tag{42}$$

Eqs. (41) and (42) are used to update the multipliers with the given parameter $\theta_{ii'}^{m} \in (0,2]$ regarding the binary variables and continuous variables, respectively. The iteration is represented by the superscript m. To ensure convergence, the value of the $\theta_{i,i'}^{m}$ should be shrunken by $\theta_{i,i'}^{m+1} = \alpha\theta_{i,i'}^{m}$ where $\alpha \in (0,1)$ if there is no improvement in the final solution; Otherwise, remain $\theta_{i,i'}^{m+1} = \theta_{i,i'}^{m}$ and start the next iteration.

5 | RESULTS AND DISCUSSION

5.1 | Computational Performance

Both the deterministic problem and the MSSP problem are solved in GAMS 42.5.0 on Windows 11 with Intel(R) Core (TM) i7-9700 CPU @3.00GHz and 16GB memory. The model statistics and computational results are shown in Tables. 2 – 3, respectively.

Table.2 Model statistics.

Problem	# of continuous variable	# of binary variable	# of constraints
Deterministic model	20,597	7,146	17,122
MSSP	11,986,305	459,264	16,011,202

Table.3 Computational results for both models.

Problem	Solver	CPU time /s	Gap /%	Objective /M$*
Deterministic model	CPLEX	3600.0	0.06	-1020.85
	Gurobi	137.5	0.01	-1020.85
MSSP	CPLEX	3600.0	/	/
	Gurobi	3600.0	13.1	-21235.2
	Lagrangean decomposition	1822.4	0.1	-24412.7

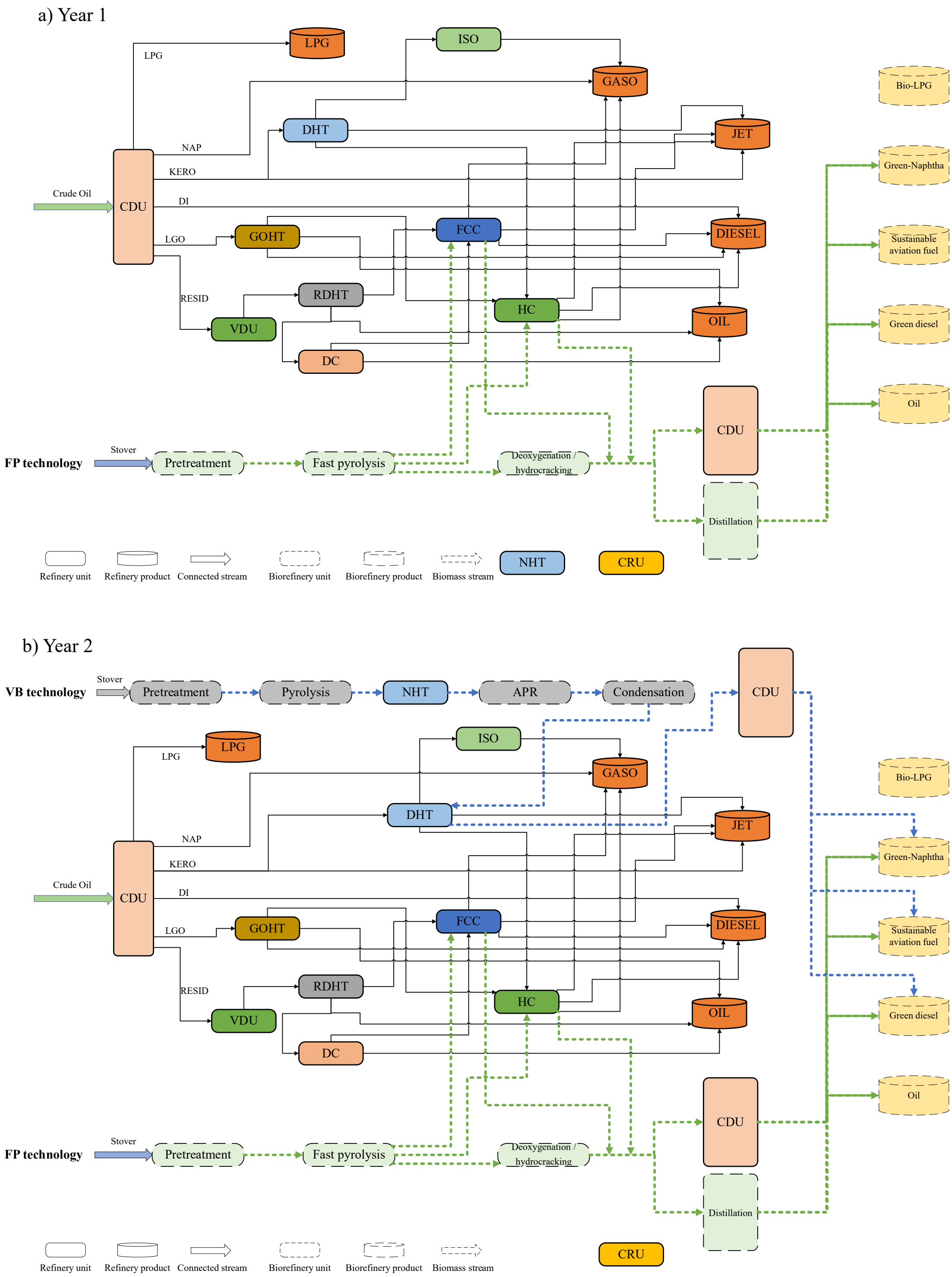
*Since the cost minimization objective is considered, its opposite value corresponds to total profit.

The deterministic model consists of 20,597 continuous variables, 7,146 binary variables, and 17,122 constraints. It only takes 137.5 seconds to solve such a problem to a gap of 0.01% with Gurobi, while CPLEX could not converge within the maximum CPU time of 3,600 seconds and remains at a gap of 0.06%. After the extension into the MSSP problem, the scale of the model greatly increases. The MSSP model consists of 11,986,305 continuous variables, 459,264 binary variables, and 16,011,202 constraints. With the proposed formulation, the scale of the MSSP increases exponentially with the number of scenarios.

To solve such an MSSP problem, the commercial solver CPLEX could not even obtain a feasible solution within 3,600 s, while Gurobi remains at a large gap of 13.1%. Applying the Lagrangean decomposition algorithm, the MSSP problem is solved to an optimality gap of 0.1% in 30 minutes. The algorithm obtains a profit of 24,412.7 M$ which is larger than the profit of 21,235.2 M$ from the solver Gurobi. The UB decreases gradually with the iteration while the LB stays almost the same. The algorithm converges to the desired gap of 0.1% with 2 iterations.

5.2 | Results of deterministic model and MSSP

The results from the deterministic model, which yields a profit of 1,020.85 M$, provide detailed retrofitting operations each year. Overall, biomass-based technologies, HEFA, VB, FP, and GFT are selected in the final biorefinery to produce the desired products. The main units are constructed gradually year by year. The flowsheets in year 1, year 2, year 5, and year 9 are displayed in Fig. 6.



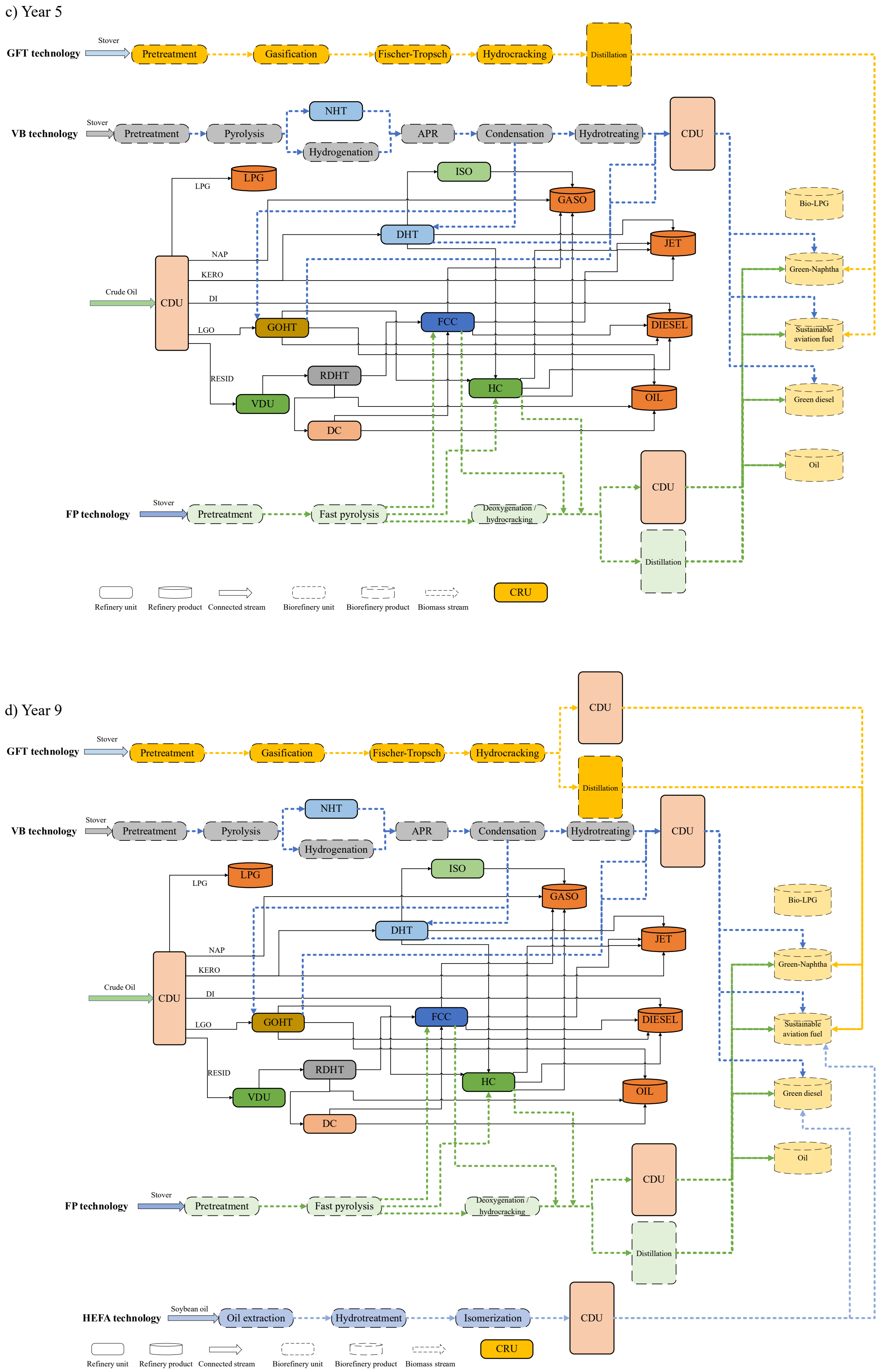


Fig. 6. Retrofitted flowsheet of the biorefinery over planned years.

In the first year, the refinery units CRU and NHT are left out from the crude refinery, and technology FP is constructed to process corn stover. Since the FP technology can utilize the existing FCC and HC units for the hydrocracking process, this technology is able to have a larger capacity to process the biomass feedstock compared to others. In addition to that, a new hydrocracking unit with a capacity of 273.5 kT/a is constructed so that a total capacity of 1,363 kT/a is obtained to handle the biomass. The capacity of the FP technology is then expanded to 1727.6 kT/a in the next year by enlarging the hydrocracking unit and then remains the same in the following years. By incorporating the FCC and HC units, the constructed hydrocracking step only needs a capacity of 471.4 kT/a in the second year and 571.4 kT/a in the fifth year, which reduces the total cost. It should be mentioned that the biomass stream after the hydrocracking step, is distilled in both the refinery CDU and constructed distillation unit to obtain the final products.

As the demand for biomass products increases, the VB technology is then selected as a second alternative. The refinery units NHT and DHT are utilized in VB technology for the hydrotreating steps sequentially to make up a capacity of 658.9 kT/a in the second year. In the third year, the GOHT unit is also implemented in the final hydrotreating step along with DHT. A newly constructed hydrotreating unit is implemented for the hydrotreating step along with NHT, providing a capacity of 1510.0 kT/a. In the following years, the capacity increases to 1877.9 kT/a. For the VB technology, the refinery CDU is utilized to separate the final biomass products for all the time periods. These units are used to update the biomass stream within year 3 to year 7 before the other technology GFT and HEFA are implemented. In the fifth year, the GFT technology is constructed with totally new processing units, providing a capacity of 1500 kT/a at the beginning. The capacity increases to 2838.9 kT/a within the following years. From the fifth year and seventh years, the biomass stream is all distilled in the exclusive distillation unit, while after that, the refinery CDU separates the final products as a supplement as shown in the flowsheet in year 9. In the last two years, the HEFA technology is used to produce biomass products while some units of HEFA are constructed in the fourth year. The HEFA units are all new units except the final distillation unit. Besides, in the ninth year, parts of the biomass stream from GFT are also processed in the CDU.

Overall, from the solution, the FP, VB, GFT, and HEFA are selected to process the biomass by utilizing the existing refinery units. These technologies are constructed in sequence to satisfy the increasing product requirements over the time horizon. Within the four alternatives, the FP and GFT decide to construct their distillation unit in addition to using the refinery distillation unit. The GFT and HEFA are constructed with new units rather than using refinery operation units for the main steps. Although the technologies may be used in later years, the processing units can be constructed earlier, releasing the benefit of long-term optimization, such as the HEFA technology. Regarding the FP and VB, the possibility to process biomass streams in the respective hydrotreating units from the refinery could help reduce the total cost, making these technologies more competitive than other technologies.

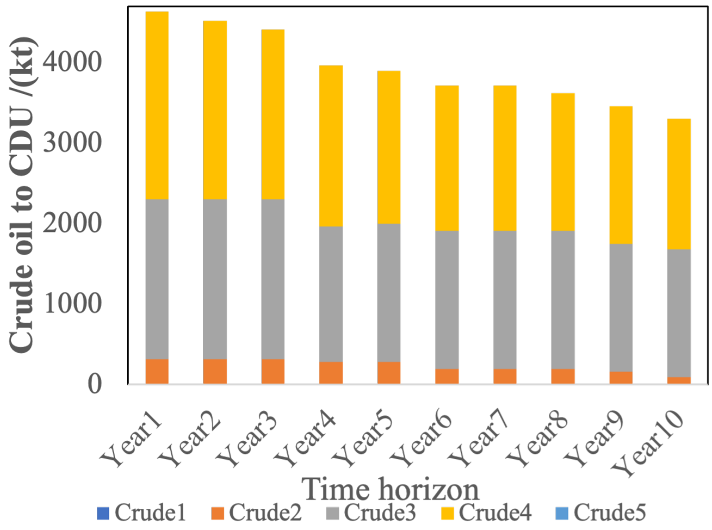


Fig. 7. Processed crude oil over the time horizon.

It is also apparent that in the retrofitted biorefinery, crude oil is still processed as the raw materials to produce fuels. Among the five potential crudes, crudes 2, 3, and 4 are selected for the entire time horizon as shown in Fig. 7. In general, the total amount of crudes to be processed in the refinery decreases over the planned years. From the first year to the third year, crude 4 is reduced gradually as the FP and VB are constructed. In the fourth year, the VB technology expands its capacity so that less crude is needed to process. Although the GFT technology is constructed in the fifth year, the processed crude remains almost the same cause the GFT technology does not utilize any existing refinery unit. The crudes keep almost the same except for the last two years when the HEFA technology is implemented. Since the refinery CDU is used to separate the products from GFT and HEFA, fewer crudes can be processed in such units. Overall, the demand for crude is decreasing over the years by retrofitting.

The final distribution of crude products and bioproducts is shown in Figs. 8 and 9. As the processed crudes decrease over the planned years, the crude products also decrease gradually, especially jet fuel and diesel, as shown in Fig. 9. On the opposite, more and more bio jet fuel (aviation fuel) is produced in the time periods, reaching to production of 901.9 kT in the last year. Also, the distribution of jet fuel, along with diesel and gasoline over the time periods are presented in Fig. 10. It is quite apparent that the proportion of biomass jet fuel (aviation fuel) is increasing over the years, reaching 70.51%. It is the same for biomass gasoline (Green naphtha) which is getting a higher biomass percentage. The production of crude gasoline decreases for the last two years since the CDU is used to distillate more biomass products from the HEAF process. Fewer crudes can be processed through the CDU. For green diesel, it shows a rapid decrease from the sixth year to the seventh year. Because this year, a vast amount of biomass in the VB process is transferred to the GFT process which does not produce green diesel. This change occurs because the GFT provides a higher yield of aviation fuel so that the demand can be satisfied. While considering the increasing demand for diesel, more biomass feedstock is processed in VB to obtain green diesel in the following years, leading to a higher percentage.

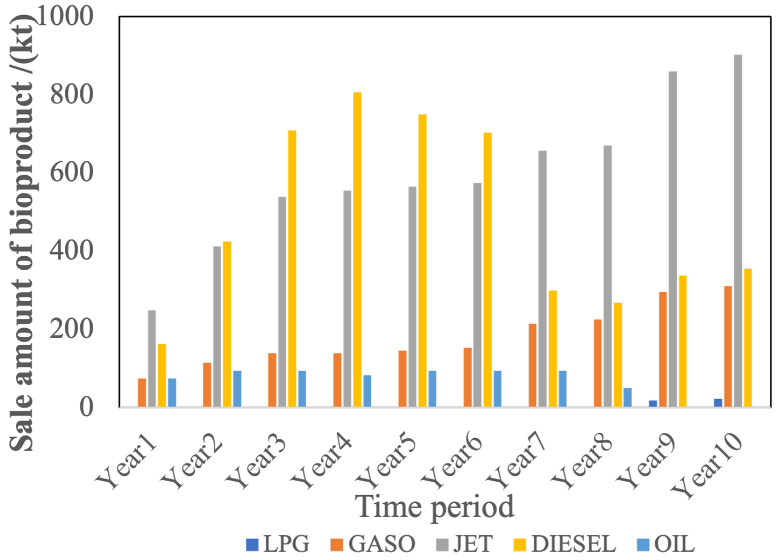


Fig. 8. Sale of bioproducts over the time horizon.

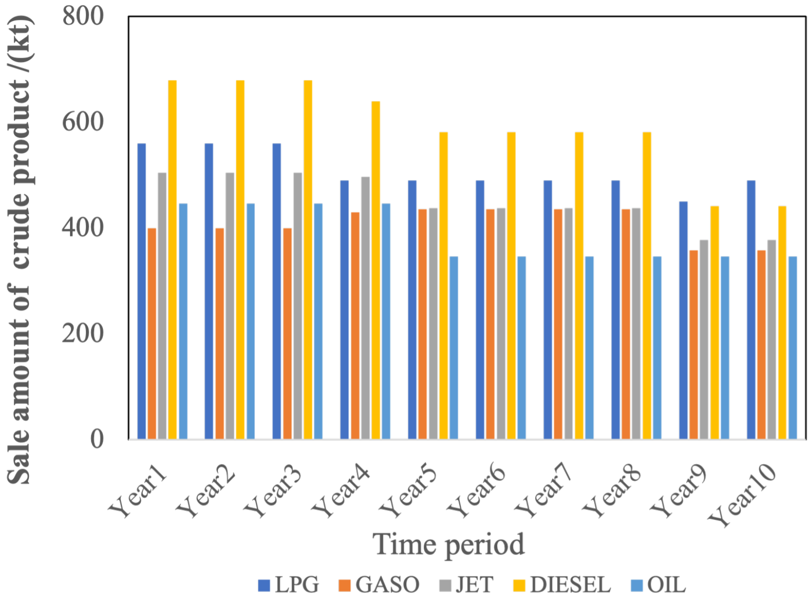


Fig. 9. Sale of crude products over the time horizon.

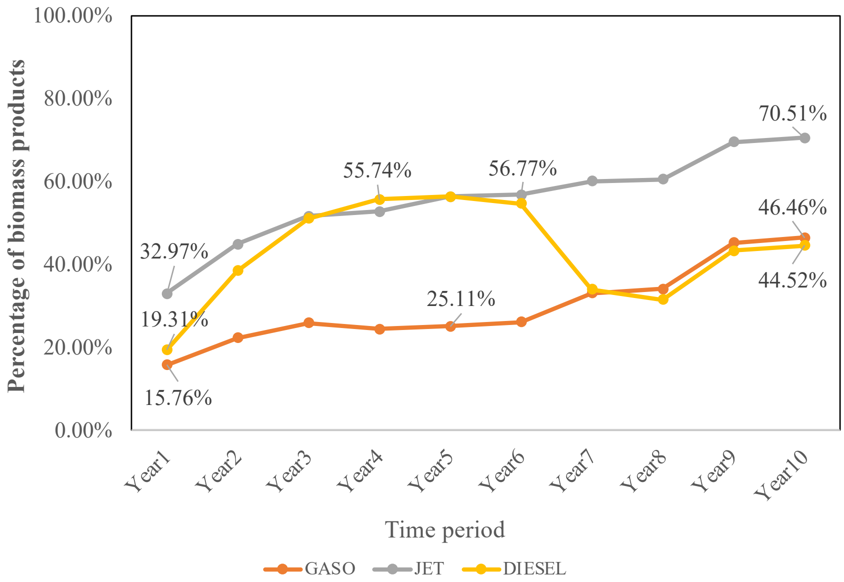


Fig. 10. Percentage of biomass products over the time horizon.

Regarding the MSSP model, the retrofitting problem is optimized under the possible endogenous uncertainty and exogenous uncertainty. The statistics among the scenarios are presented in Table. 4.

Table.4 Statistics of Results from MSSP

Technology	Scenarios selecting technology	Technology	Scenarios selecting technology
HEFA	28	DSHC	0
VB	64	FP	64
ATJ	0	GFT	36

For a total of 64 scenarios divided by the endogenous uncertainty, VB and FP are all selected as the main process to produce biomass-based hydrocarbons, while ATJ and DSHC are not. Compared to VB and FP, the higher expense and lower yield of ATJ and DSHC prevent their applications. To compensate for the production demands, GFT and HEFA are the backup biomass-based technologies to be implemented in later years. The GFT is preferred since it is selected in 36 scenarios while HEFA is selected in 28 scenarios. The results illustrate that the FP and VB are more competitive than other alternatives. The final flowsheets for scenario 4 and scenario 14 are demonstrated in Figs. 11 – 12 as examples. Compared to the deterministic results, the GFT technology is skipped in scenario 4 since the uncertain yield of FP is assumed to be higher, as shown in Fig. 11. Due to that, the FCC is retrofitted entirely in the FP technology to process the biomass. No crudes are imported into the FCC unit anymore in such a scenario. Besides, all the selected technologies utilize the CDU to separate the final biomass products leading to a lower capacity for crudes. The CRU unit is used to update the naphtha stream from CDU which is then transported into the ISO unit and finally blended as the gasoline. It should also be mentioned that, in such a scenario, a hydrotreating unit, RDHT is further utilized in VB technology for the final hydrotreating process. In scenario 14 shown in Fig 12, which assumes a higher yield for VB technology, the HEFA is not needed to increase the total capacity for the biomass.

In this scenario, the FP, VB, and GFT are selected as the potential technologies for the biorefinery. The FP utilizes the FCC totally and constructs a new distillation unit to separate the final products. The GFT is entirely constructed except for the final distillation unit. Regarding the VB technology, the NHT could process the crude stream due to the higher yield of VB, which is the main difference from the deterministic model.

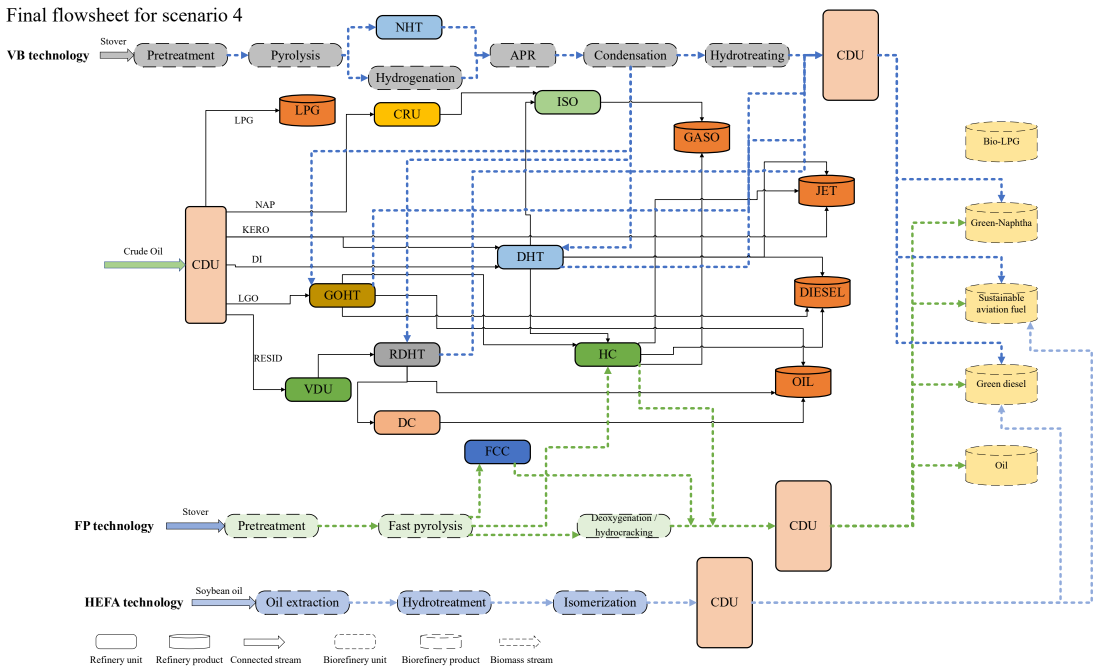


Fig. 11. Retrofitted flowsheet of the biorefinery for scenario 4.

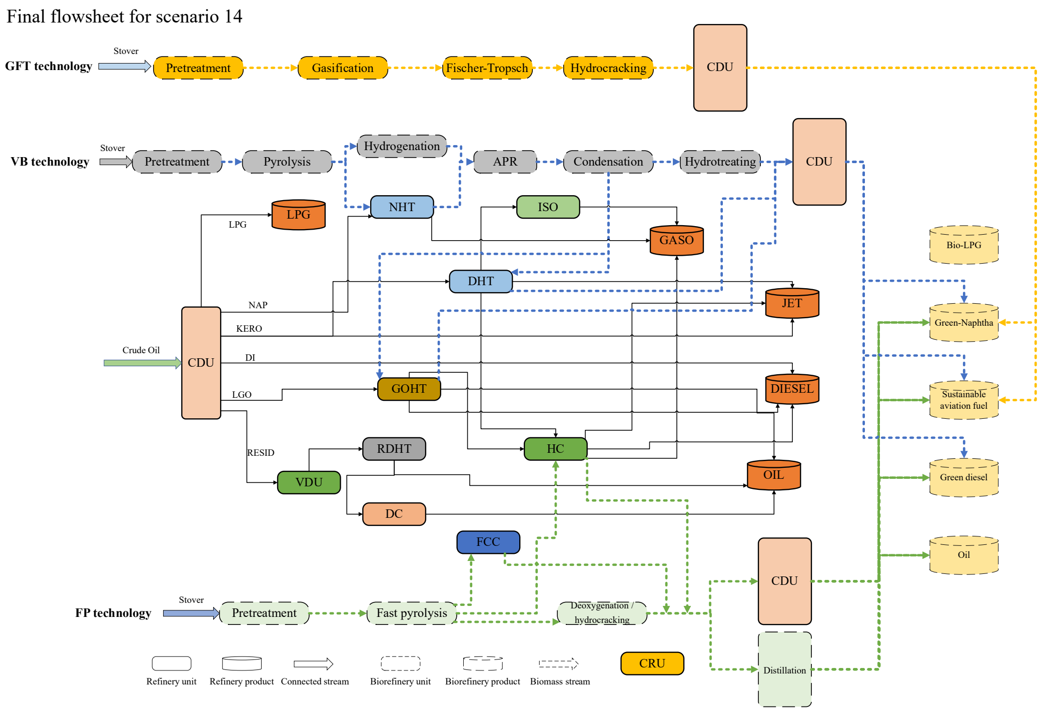


Fig. 12. Retrofitted flowsheet of the biorefinery for scenario 14.

To evaluate the potential advantage of the MSSP, the value of the stochastic solution (VSS) is also calculated by solving the deterministic problem at each stage.[44] The definition of VSS and $\overline{VSS}$ are presented as follows.

$$VSS = z^{DP} - z^{MSSP}$$

$$\overline{VSS} = (z^{DP} - z^{MSSP})/\, z^{DP}$$

The objective z^{DP} is obtained from solving the MSSP problem stage by stage iteratively. Each stage is formulated as a deterministic problem with the strategic decisions fixed at the values from the MSSP solution. The uncertain demand parameters are set to the expected values. This yields a profit of 24,153.6 M$ as the expected objective of all the scenarios. The objective z^{MSSP} is obtained from the MSSP model which yields a profit of 24,402.6 M$. The VSS equals 249 M$ (since the objective is obtained with the negative profit), and therefore the $\overline{VSS}$ is 1.03%, which indicates the benefit of implementing stochastic programming for this problem.

6 | CONCLUSION

This paper presents a retrofit problem from a conventional refinery into a biorefinery by utilizing the existing operational units in six potential alternative biomass-based technologies. The deterministic problem is formulated as a multiperiod MILP model over ten years. The problem is next extended into a MSSP model under both endogenous yield and exogenous demand uncertainty by dividing the decisions into strategic and operational decisions. The strategic decisions are assumed to be related to endogenous yield uncertainty and are determined to ensure the feasibility of operation regarding the exogenous demand uncertainty revealed at each stage independently. The MSSP is solved to optimality with a Lagrangean decomposition algorithm.

The results show that among the alternatives, Virent's BioForming (VB) and fast pyrolysis (FP) are the most competitive technologies when the corn stover is considered as the feedstock since the refinery units can be used as the hydrotreating and hydrocracking steps so that capital costs can be saved. With stochastic programming, a benefit of 249 M$ is obtained under the evaluation of the value of the stochastic solution. Future work on the problem addressed in this paper can be focused on the modeling of detailed blending of the hydrocarbons, which are mixed for co-processing. A more detailed economic evaluation of the technology can also be included to make the solution more rigorous.

Appendix

Conversion of the property and property index

Property	Property index	Blending bias
Specific Gravity (SG)	/	Volume
Sulfur Content (S)	/	Mass
Research Octane Number (RON)	RONI=651*z^3-1552.9*z^2+1272*z-299.5 (z=RON/100)	Volume

Cetane Number (CN)	CI=0.72*(API)*(1.8AP+32)/100+10 (AP : Amine point; API = 141.5/SG-131.5)	Volume
Reid Vapor Pressure (RVP)	RVPI=RVP^1.25	Volume
Flash Point (FP)	FPI=-6.1188+2414/(FP-426)	Volume
Smoking Point (SP)	SPI=-362+[2300/ln(SP)]	Volume
Pour Point (PP)	PPI=316200*exp[12.5*ln(0.001(PP+459.67))]	Volume

NOMENCLATURE

Abbreviation

CDU	Crude Distillation Unit
VDU	Vacuum Distillation Unit
NHT	Naphtha Hydrotreating Unit
DHT	Diesel Hydrotreating Unit
GOHT	Gasoline Hydrotreating Unit
RDHT	Residue Hydrotreating Unit
ISO	Isomerization Unit
CRU	Continuous Reforming Unit
FCC	Fluid Catalytic Cracking Unit
HC	Hydrocracking Unit
DC	Delayed Coking Unit
LPG	Liquified Petroleum Gasoline
GASO	Gasoline
JET	Jet Fuel (Aviation Fuel)
DIESEL	Diesel
OIL	Fuel Oil
NAP	Naphtha Stream
KERO	Kerosene Stream
DI	Diesel Stream
LGO	Light Gas Oil
RESID	Residue Oil

Sets and Indices

T	Set for time period
C	Set for crude oils
B	Set for biomass materials
K	Set for alternative technology
P	Set for final products
U	Set for processing units
S	Set for streams

Superscript

cru	Crude oil
bio	Biomass
$equi$	Capacity of constructed unit
sub	Capacity of substituted unit
up	Upper bound
lo	Lower bound
$oper$	Operation
exp	Expansed capacity
min	Minimum parameter
max	Maximum parameter

Parameters

pr	Price parameter
co	Capacity cost parameter
Inv	Inventory bound or available amount
Cap	Capacity parameter
$Yield$	Yield parameter
a	Capacity bound parameters
E	Property index parameter
$demand$	Demand parameter

Binary variables

$y_{k,u,l}^{equi}$	Piecewise linearization interval *l* for unit *u* of technology *k*
$y_{u,k,u'}^{sub}$	Substitution of refinery unit *u* to biorefinery unit *u'* of technology *k*
$y_{t,c}^{cru}$	Selection of crude oil *c* at year *t*
$y_{t,u,k,u'}^{nonco}$	Non-co-processing substitution for unit *u* as unit *u'* of technology *k* at year *t*
$y_{t,u,k,u'}^{co}$	Co-processing substitution for unit *u* as unit *u'* of technology *k* at year *t*
$y_{t,k,b}^{feed}$	Selection of biomass feedstock *b* for technology *k* at year *t*
$y_{t,k}^{op}$	Operation for technology *k* at year *t*
$y_{t,k,u}^{exp}$	Expansion decision of unit *u* of technology *k* at year *t*

Continuous variables

$cost^{feed}$	Material purchase cost

$cost^{equi}$	Unit construction cost
$cost^{oper}$	Unit operation cost
$income^{sale}$	Sale income of final products
$F_{t,c}^{in}$	Flowrate of crude oil *c* at year *t*
$F_{t,b}^{in}$	Flowrate of biomass *b* at year *t*
$F_{t,u}^{in}$	Flowrate to unit *u* at year *t*
$F_{t,p}^{sale}$	Sale amount of final product *p* at year *t*
$F_{t,c,w}$	Flowrate of swing-cut *w* of crude oil *c* at year *t*
$F_{t,c,w,s}$	Flowrate of swing-cut *w* to stream *s* of crude oil *c* at year *t*
$F_{t,c,s}^{out}$	Flowrate of stream *s* from crude *c* at year *t*
$F_{t,c,s,u}$	Flowrate of stream *s* to unit *u* from crude *c* at year *t*
$F_{t,c,s,p}$	Flowrate of stream *s* to product *p* from crude *c* at year *t*
$F_{t,u',s,u}$	Flowrate of stream *s* from unit *u'* to unit *u* at year *t*
$F_{t,u,s}^{out}$	Flowrate of stream *s* from unit *u* at year *t*
$F_{t,u,s,p}$	Flowrate of stream *s* to product *p* from unit *u* at year *t*
$F_{t,k,b}^{in}$	Flowrate of feedstock *b* to technology *k* at year *t*
$ca_{t,k,u}$	Capacity of unit *u* in technology *k* at year *t*
$ca_{t,k,u}^{exp}$	Expanded capacity of unit *u* in technology *k* at year *t*
$\lambda_{k,u,l}^{up}$	Linear weight of upper capacity in piecewise interval *l* for unit *u* in technology *k*
$\lambda_{k,u,l}^{lo}$	Linear weight of lower capacity in piecewise interval *l* for unit *u* in technology *k*
$F_{t,k,b,u}^{in}$	Flowrate of feedstock *b* to unit *u* of technology *k* at year *t*
$F_{t,k,b,u,s}^{out}$	Flowrate of stream *s* from unit *u* of biomass *b* in technology *k* at year *t*
$F_{t,k,u,u'}^{sub}$	Flowrate of stream from unit *u* to refinery unit *u'* in technology *k* at year *t*
$F_{t,k,u}^{new}$	Flowrate of stream to construct unit *u* in technology *k* at year *t*

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Supporting information

Optimal Retrofitting of Conventional Oil Refinery into Sustainable Bio-refinery under Uncertainty

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Table 1. Demand parameters for the main products (kt/a)

	Gasoline		Jet fuel		Diesel	
	Lower	Upper	Lower	Upper	Lower	Upper
Year 1	1098.45	700.00	2637.12	1000.00	1608.26	800.00
Year 2	1109.43	800.00	2663.5	1500.00	1624.34	1100.00
Year 3	1120.53	800.00	2690.13	1500.00	1640.59	1100.00
Year 4	1131.73	800.00	2717.03	1500.00	1656.99	1100.00
Year 5	1143.05	800.00	2744.20	1500.00	1673.56	1100.00
Year 6	1154.48	800.00	2771.64	1500.00	1690.30	1100.00
Year 7	1166.03	800.00	2799.36	1500.00	1707.20	1100.00
Year 8	1177.69	800.00	2827.35	1500.00	1724.27	1100.00
Year 9	1189.46	800.00	2855.63	1500.00	1741.52	1100.00
Year 10	1201.36	800.00	2884.18	1500.00	1758.93	1100.00

*The lower demand is used to generate the scenarios by multiplying 0.9, 1.0 and 1.1 for the main products in each year.

Table 2. Price parameters for the crude products ($/t)

	LPG	Gasoline	Jet fuel	Diesel	Oil
Year 1	647.61	1162.95	415.34	1190.64	542.32
Year 2	634.66	1139.69	407.03	1166.83	531.47
Year 3	621.96	1116.90	398.89	1143.49	520.84
Year 4	609.53	1094.56	390.91	1120.62	510.43
Year 5	597.33	1072.67	383.10	1098.21	500.22
Year 6	585.39	1051.21	375.43	1076.24	490.21
Year 7	573.68	1030.19	367.93	1054.72	480.41
Year 8	562.21	1009.59	360.57	1033.62	470.80
Year 9	550.96	989.39	353.36	1012.95	461.39
Year 10	539.94	969.61	346.29	992.69	452.16

Table 3. Price parameters for the biomass products ($/t)

	LPG	Gasoline	Jet fuel	Diesel	Oil
Year 1	905.26	1098.45	2637.12	1608.26	806.65
Year 2	914.31	1109.43	2663.50	1624.34	790.51
Year 3	923.45	1120.53	2690.13	1640.59	774.70
Year 4	932.69	1131.73	2717.03	1656.99	759.21
Year 5	942.01	1143.05	2744.20	1673.56	744.02
Year 6	951.43	1154.48	2771.64	1690.3	729.14
Year 7	960.95	1166.03	2799.36	1707.2	714.56
Year 8	970.56	1177.69	2827.35	1724.27	700.27
Year 9	980.26	1189.46	2855.63	1741.52	686.26
Year 10	990.07	1201.36	2884.18	1758.93	672.54

Table 4. Yield parameters for the alternative biomass technology (Adapted from the reference[1–3])

	LPG	Gasoline	Jet fuel	Diesel	Oil
HEFA	0.07142857	0.08571429	0.58571429	0.27142857	
VB		0.03448276	0.17241379		
ATJ		0.01538462	0.10769231	0.03333333	
DSHC	0.01785714	0.02857143	0.05357143	0.00714286	
FP		0.03103448	0.09310345	0.06206897	0.03448276
GFT		0.03953488	0.11395349		

*Multiply 0.9 and 1.1 with the yield of jet fuel respectively to generate the uncertain yield uncertainty.

Table 5. Referred Construction cost for the alternative technology (Adapted from the reference[1–3])

HEFA		VB		ATJ	
Unit	Cost (10^4 $)	Unit	Cost (10^4 $)	Unit	Cost (10^4$)
Oil extraction	3573.938	Pretreatment	5718.303	Pretreatment	7952.019
Hydrotreating	6969.176	Hydrolysis	10185.73	Hydrolysis	9560.266
Isomerization	536.091	Hydrogenation	10453.76	Fermentation	8488.08
Distillation	1697.275	APR	20103.44	Dehydration	1518.923
		Condensation	2233.715	Oligomerization	1518.923
		Hydrotreating	10185.73	Hydrotreating	1518.923
		Distillation	959.0552	Distillation	1085.247

DSHC		FP		GFT	
Unit	Cost (10^4 $)	Unit	Cost (10^4 $)	Unit	Cost (10^4 $)
Pretreatment	15993.38	Pretreatment	7147.863	Pretreatment	8666.83
Hydrolysis	14117.04	Fast pyrolysis	29038.23	Gasification	6969.176

Fermentation	7058.52	Hydrocracking	14385.13	Fischer-Tropsch	11257.92
Isomerization	20103.44	Distillation	608.8738	Hydrocracking	5539.604
Distillation	719.2914			Distillation	763.4584

*The capacity bias is 1000 kt/a and the cost function is (capacity/capacity bias)^0.6 = (cost/cost bias)

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