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Integrated Ex-Ante Life Cycle Assessment and Techno-Economic Analysis of Biomass Conversion Technologies Featuring Evolving Environmental Policies

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ABSTRACT

Biorefineries can reduce carbon dioxide emissions while serving the global chemical demand market. Governments are also using carbon pricing policies, such as carbon taxes, cap-and-trade models, and carbon caps, as a strategy to reduce emissions. The use of biomass feedstocks in conjunction with carbon capture usage and storage technologies are mitigation strategies for global warming. Businesses can invest in these technologies to accommodate the adoption of these policies. Rapid action is necessary to halt global warming, which results in aggressive policies. In this work, a multi-period process design and planning problem is developed for the design and capacity expansion of biorefineries. The three carbon pricing policies are integrated into the model and parameters are selected according to the aggressive scenario denoted by the Paris Agreement. The results show that the cap-and-trade policy achieves a higher net present value evaluation over the carbon tax model across all pareto points due to the flexibility of the allowances in the cap-and-trade policy. The carbon cap model substantial investments are required in carbon capture technologies to adhere to the emissions constraints.

Keywords: Biomass, Life Cycle Analysis, Technoeconomic Analysis, Technoeconomic Analysis, Process Design

INTRODUCTION

CO_2 emissions from energy combustion and industrial processes have risen from 24.9 Gt CO_2 to 36.8 Gt CO_2 from 2000 to 2022[1]. The Intergovernmental Panel on Climate Change (IPCC) reported that urgent action is necessary to curb global warming to 1.5°C[2]. Towards that end, scientists and policymakers are developing solutions to mitigate CO_2 contributions to the global warming crisis.

Traditional chemical manufacturing uses petroleum-based feedstocks, which are unsustainable resources and result in high CO_2 emissions. In an effort to reduce reliance on petroleum-based feedstocks, scientists have been researching lignocellulosic biomass as a feedstock alternative. Lignocellulosic biomass is an abundant resource and has the potential to be sustainable with low emissions. The biorefinery concept proposes that each major component from lignocellulosic biomass, i.e., cellulose, hemicellulose, and lignin, can be fractionated and valorized into chemicals, like petroleum refinery and chemical plant operations. Biorefineries supports decarbonization by transitioning towards a sustainable feedstock and lower emissions processes.

Significant research has been conducted in the Carbon Capture, Utilization, and Storage (CCUS) field that aims to reduce the amount of CO_2 currently emitted by industrial processes and capture CO_2 already existing in the atmosphere. For example, Yusuf et al. evaluated the economic feasibility of producing soda ash from CO_2 heavy flue gas generated from power plants, a Carbon Capture and Utilization (CCU) technology[3]. Wang et al. performed a technoeconomic analysis on the sequestration of CO_2 flue gas from power plants via compression and storage, a Carbon Capture and Storage (CCS) technology[4].

Governments are increasingly leveraging environmental policies to reduce CO_2 emissions. As of 2022, 23%

of all CO_2 emissions are under some form of carbon pricing policy[5]. Fifty-two countries enforce a carbon tax, Emissions Trading System (ETS), or both policies[5]. Twenty countries are currently considering the implementation of these policies as they can provide not only environmental but also social and economic benefits[5]. Under a carbon tax policy, carbon dioxide emitters are charged a financial penalty per ton of CO_2 emitted. An ETS is a system enforcing a cap-and-trade model where the government provides allowances, an amount of permitted CO_2 emissions, for manufacturers. They can purchase additional allowances or sell unused allowances on an open market. Benchmarks have been set via carbon pricing to limit global warming to 2°C. According to the Paris Agreement, emission levels should be reduced by 45% by 2030 and reach net-zero carbon emissions by 2050[5]. An additional benchmark provided by the World Bank states that carbon pricing should be between 61 and 122$ by 2030[5].

Superstructure optimization is used as a framework for exploring multiple process design alternatives. Luo et al. utilized neural networks to model the biorefinery flexibility index facilitating operational flexibility constraints in superstructure optimization[6]. Multi-period optimization can be used for considering planning problems over a long-time horizon. Sabet et al. used a multi-period formulation to model a global manufacturing capacity management problem[7]. These two approaches can be integrated with environmental policy to optimize process designs.

This work incorporates the benchmarks provided by the World Bank and IPCC into a multi-period biorefinery design and optimization problem[2, 5]. Three different carbon emissions policies, namely carbon cap, cap and trade, and carbon tax, are considered as constraints in the formulation. Pareto fronts are constructed for economic and environmental objective functions.

MULTI-PERIOD PROGRAMMING FOR BIOREFINERY

The multi-period programming formulation is utilized for the long term biorefinery construction and expansion optimization problem. The planning horizon is set for thirty years corresponding to the Paris Agreement goals. Each time period represents one year. In the first year, an initial biorefinery is constructed. In each subsequent time period, the biorefinery can experience capacity expansion or the construction of new units. The problem is constrained by three environmental policies that are increasingly restrictive over each time period to match the IPCC and Paris Agreement benchmarks while maximizing net present value.

A superstructure approach is used. In this work, the superstructure represents all process alternatives consisting of chemical transformations and separation sequences. The reactions were selected to represent a broad range of chemicals, which is displayed in Figure 1. Commodity chemicals, such as ethanol, and biomass platform chemicals, such as furfural, were included. Drop-in chemicals, such as para-xylene, and biomass derived alternatives, such as furan-dicarboxylic acid, were also included. Different separation steps were considered consisting of crystallization, distillation, extraction, membrane separation, and pervaporation. Shortcut methods and surrogate models are used to characterize the utility usages. Carbon capture storage and carbon capture and utilization technologies were also incorporated into the superstructure to accommodate the dynamic environmental policies.

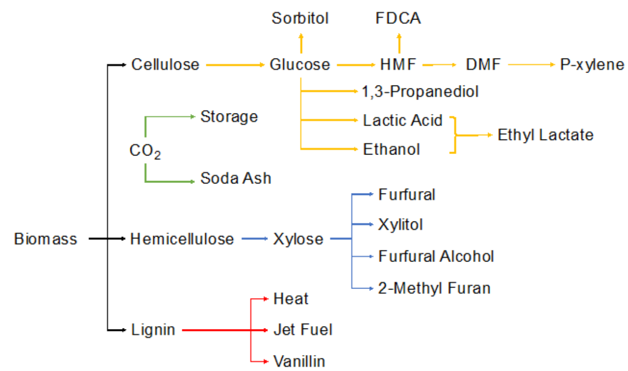

Figure 1. Biorefinery superstructure with CCUS technologies.

Objective Functions

The objective of the optimization problem is to maximize net present value (NPV) and minimize cumulative emissions (CE) while adhering to the carbon pricing policies. The net present value calculation is shown in Equation (1) where ir represents the interest rate, t represents the time period; IC_t represents the capital investment in time period t; R_t represents the product revenue in time t; O_t represents the operating cost in time t; and $C_{CO2,t}$ represents the carbon dioxide cost in time period t.

$$NPV = \sum_{t \in T} (1 + ir)^{-t} \{-(IC_t - \mathrm{IC}_{t-1}) + R_t - O_t \pm C_{CO2,t}\} \quad (1)$$

The power law model in Equation (2) captures the capital costs where a_u and b_u are parameters for unit operation u, and $x_{u,t}$ represents the cumulatively capacity of unit u in period t. The cost of capacity expansion in time period t is captured as the difference between the cost of a plant with the cumulative capacity and the cost of the plant in the previous expansion period.

$$IC_t = \Sigma_{u \in U} a_u \left(x_{u,t}\right)^{b_u}, \mathrm{t} > 1 \quad (2)$$

The revenue, R_t, generated in time period t by the products are captured in Equation (3), where $b_{i,t}$ is the amount of chemical i produced in time period t, and C_i represents the cost of chemical i.

$$R_t = \sum_{i \in I} b_{i,t} C_i \tag{3}$$

The operating cost, O_t, in time period t is captured in Equation (4), where $f_{j,t}$ is the operating level of unit operation j in time period t; C_j is the unit cost of running unit j; $E_{w,tt}$ is the energy usage of utility w; C_w is the unit cost of operating utility w; and fcf is the fixed cost factor.

$$O_t = \sum_{j \in j} f_{j,t} C_j + \sum_{w \in W} E_{w,t} C_w + IC_t(fcf) \tag{4}$$

The environment impact calculation is based on a cradle-to-gate life cycle assessment. The system boundary is depicted in Figure 2 and considers biomass transportation, raw material production, utilities, combustion products, landfill, and wastewater treatment. Biomass is assumed to be carbon neutral. The data for the calculations are obtained from the Ecoinvent v.3.8 database, and the Global Warming Potential (GWP) indicator from the ReCipE2016 impact assessment method is used[8, 9].

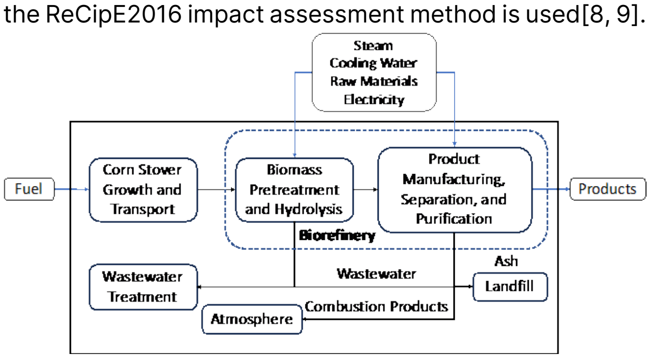

Figure 2. System boundary depicted for environmental impact calculations. Biomass is transported to the biorefinery. Raw materials and utilities are imported into the biorefinery for chemical production. Wastewater is exported for wasterwater treatment. Emissions from the combustion of lignin to the atmosphere and the resulting ash sent to the landfill are included.

The environmental impact in time period t, TE_t, is given by Equation (5) where GWP_w represents the GWP of utility w; $b_{ww,t}$ represents the amount of waterwater generated in time period t; GWP_{ww} represents the GWP of wastewater treatment; $f_{rm,t}$ represents the amount of raw material rm used in time period t; $b_{Ash,t}$ represents the amount of ash generated in time period t; GWP_{Ash} represents the GWP of sending the ash to the landfill; b_{comb} represents the combustion products in time period t; and GWP_{comb} represents the GWP of the combustion product mixture.

$$TE_t = \sum_{\mathrm{w}} E_{w,t}\,\mathrm{GWP_w} + b_{ww,t} GWP_{ww} + \sum_{rm \in RM} f_{rm,t} GWP_{rm} + \mathrm{b}_{Ash,t}\mathrm{GWP_{Ash}} + \mathrm{b_{comb}GWP_{comb}} \tag{5}$$

The second objective function, cumulative emissions (CE), is given by Equation (6) where TE_t represents the total emissions in time period t.

$$CE = \sum_t TE_t \tag{6}$$

In this work, it is assumed that the residence time of CO_2 emissions is longer than the planning period and, therefore, that the emissions across the time periods have equal weight.

Constraints

The processing of materials is described by the molar balance Equation (7) where $\nu_{i,j}$ represents the conversion coefficient for compound i in operation j; $f_{j,s}$ is the extent of process j in time period t; and $b_{i,t}$ is the amount of chemical i in time period t.

$$\Sigma_j \nu_{i,j} f_{j,s} = b_{i,s} \tag{7}$$

The unit operation expansion is described by Equations (8a) and (8b) where $x_{j,t}$ represents the capacity of unit operation j in time period t; where $x_{j,t}^{exp}$ the additional capacity added to unit operation j in period t; and x_j^{init} represents the initial capacity built for unit operation j.

$$x_{j,t} = x_{j,t-1} + x_{j,t-1}^{exp} \quad \forall j; t > 1 \tag{8a}$$

$$x_{j,t} = x_j^{init} \quad \forall j;\ t = 1 \tag{8b}$$

The capacity expansion is limited in its lower and upper bound as expressed in Equation (9), where $Y_{j,t}$ is a binary variable that equals 1 when there is capacity expansion; where $\mathrm{Cap^{Lo}}$ represents the minimum possible capacity expansion; and $\mathrm{Cap^{Up}}$ represents the maximum possible capacity expansion.

$$Cap^{Lo} Y_{j,t} \le x_{j,t}^{exp} \le Cap^{Up} Y_{j,t} \tag{9}$$

The capacity is limited to a fixed number of expansions represented by Equation (10), where $Y_{j,t}$ represents expansion in time period t, and $\mathrm{E_j}$ represents the number of expansions permitted for unit j.

$$\sum_t Y_{j,t} \le E_j\ \forall j \tag{10}$$

The operating level of unit j is constrained by the maximum capacity of unit j, which is expressed in Equation (11). $\mathrm{x_{j,t}}$ represents the capacity of unit j in time period t; h represents the minimum operating ratio; and $\mathrm{f}_{j,t}$ represents the operating level of unit j in time period t.

$$hx_{j,t} \leq f_{j,t} \leq x_{j,t} \quad \forall j \in J\, \forall t \in T \tag{11}$$

The plant size is limited to amount m_{bm} as expressed in Equation (12) where $x_{bm,t_{end}}$ represents the biomass feedstock, bm, processing capacity in the last period.

$$m_{bm} = \sum_{\mathrm{bm} \in \mathrm{BM}} x_{bm,t_{end}} \tag{12}$$

Environmental Constraints

The formulations for the carbon policies utilized in this work are presented below. These policies enforce environmental constraints and may affect the NPV calculation.

The carbon cap policy enforces a fixed amount of CO_2 emissions. In this work, we consider the cap to be placed on the aggregated amount of emissions in the time period of one year. The constraint is expressed in Equation (13) where TE_t represents the amount of CO_2 emitted in time period t, and TE_t^{Cap} represents the emissions cap in time period t.

$$TE_t \leq TE_t^{Cap} \quad \forall t \in T \tag{13}$$

In the cap-and-trade policy, the governing body allocates a number of allowances to manufacturers. This represents a soft emissions cap, which can be exceeded by purchasing additional allowances from other manufacturers or can be sold for profit. The constraint is expressed in Equations (14-16) where $P_{CO2,t}$ represents the price of CO_2 in time period t; $E_t{}^+$ represents the allowances purchased in time period t; $E_t{}^-$ represents the allowances sold in time period t; and TE_t^{Cap} represents the allowances provided in time period t.

$$C_{CO2,t} = P_{CO2,t}\left(E_t{}^+ - E_t{}^-\right) \tag{14}$$

$$TE_t \leq TE_t^{Cap} + E_t^+ - E_t^- \quad \forall t \in T \tag{15}$$

$$E_t^+ > 0, E_t^- > 0\ \forall t \in T \tag{16}$$

Under a carbon tax policy, manufacturers are charged per tCO_2 emitted. The total carbon tax is given by Equation (17), where $P_{CO2,t}$ represents the price of one ton of CO_2 emitted in time period t; TE_t represents the amount of CO_2 emitted in time period t; and $C_{CO2,t}$ represents the carbon tax cost associated with those emissions in period t.

$$C_{CO2,t} = P_{CO2,t} TE_t \tag{17}$$

CASE STUDY RESULTS AND DISCUSSION

The epsilon constraint method is used to construct a Pareto front for the multi-period biorefinery optimization problem. NPV and CE are the two functions considered in the bi-objective optimization. The nonlinear Equation (2) is reformulated via piecewise linearization to keep the formulation linear. Consequently, all instances of the model are formulated and solved in GAMS as a MILP using CPLEX solver on an Intel Xeon E-2247G @ 4.00 GHz CPU and 32.0 GB of RAM.

In our case study, a biorefinery is considered in McClean, IL with a plant capacity set at 2984 metric tons per year corresponding to four times the nominal corn stover production in McClean. Additional biomass can be purchased within the five closest counties within McClean. The years 2020 to 2050 are considered to represent a thirty-year time horizon with each time period having a length of one year. The carbon pricing parameters considered correspond with the aggressive scenario set by the Paris Agreement, which aims to maintain global warming below 2°C. Table 1 presents the parameter benchmarks. Linear interpolation is used to determine the parameters in the intermediate years. The carbon tax and cap-and-trade policies are evaluated by constructing pareto fronts to compare economic and environmental trade-offs. The carbon cap policy is analyzed yearly to elucidate the effects of a shrinking carbon cap.

Table 1: Carbon pricing policy parameters during milestone years

Year	Carbon Cap (%)	Carbon Tax ($/$tCO_2$)
2020	100	0
2030	45	59
2050	0	295

Figure 3 demonstrates increasing NPV with increasing CE for both cap-and-trade and carbon tax policies. For the cap-and-trade policy, the allowances provided are equal to the carbon cap parameters given in Table 1. Similarly, the carbon prices are set at the carbon tax value in Table 1. At the minimum CE point for both policies, a positive NPV exists. Across all points on the pareto front, the cap-and-trade policy results in a higher NPV than the carbon tax policy. This is a consequence of the allowances that can be sold for a profit when the carbon cap is high as well as the allowances providing tax-free emissions. Additional production incurs a larger financial penalty under the carbon tax policy, resulting in lower overall production. This is noted through the maximum profit point for the carbon tax policy having lower CE than the cap-and-trade policy.

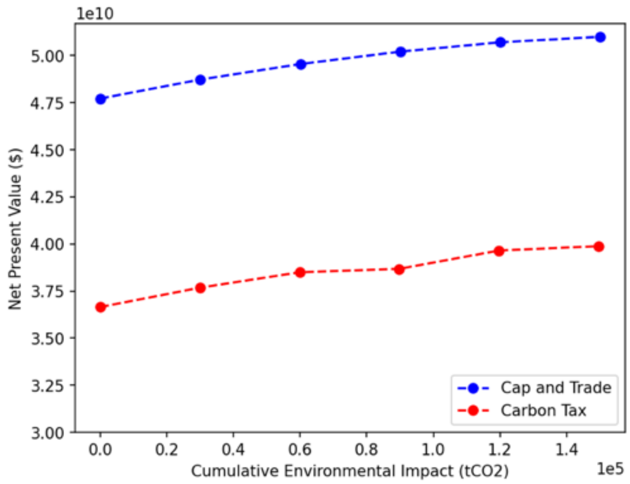

Figure 3. NPV and CE pareto curve for cap-and-trade and carbon tax policies

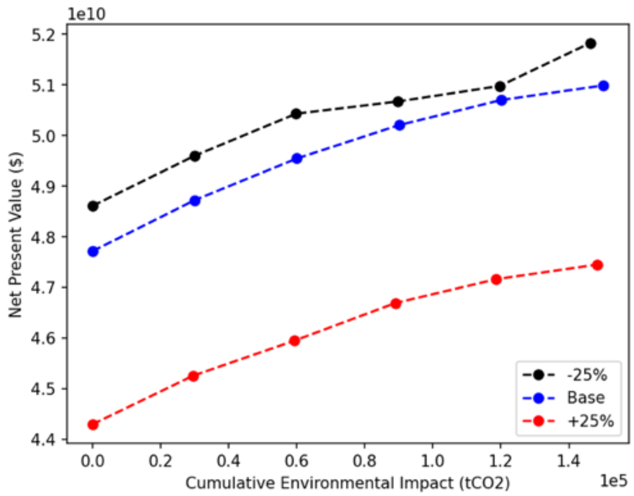

Figure 4. Sensitivity analysis for NPV and CE pareto curve for a cap-and-trade policy

A sensitivity analysis was performed for the cap-and-trade and carbon tax policies. The raw material costs were varied by 25%. Figure 4 and Figure 5 show the changes in the pareto curves for the cap-and-trade and carbon tax policies, respectively. In both policies, increasing the raw material price by 25% has a significantly greater impact than decreasing the raw material price by 25%. For the carbon tax policy, the average relative difference to the base case for the 25% increase and decrease case is 9.0% and 2.2%, respectively. For the cap-and-trade policy, the average relative difference to the base case between the 25% increase case and decrease case is 7.1% and 1.4%, respectively. The large decrease in NPV in the 25% increase case is explained by the change in production relative to the base case. In the 25% increase case, production shifts from ethyl lactate to ethanol production which has higher raw material costs. The average relative differences for the carbon tax policy are greater than those of the cap-and-trade policy because emissions are more heavily penalized under the carbon tax policy.

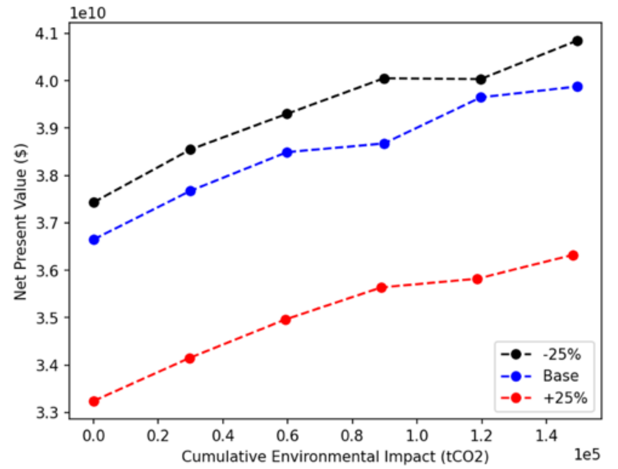

Figure 5. Sensitivity analysis for NPV and CE pareto curve for carbon tax policy

Figure 6 demonstrates the effect of an increasingly restrictive carbon cap over time. It is clear from the emissions curve that the rate of carbon dioxide reduction is greater between 2020 to 2030 than between 2030 and 2050. Despite the rapid reduction in emissions levels, the yearly profit generated is unaffected until 2029. This is a consequence of decreasing production in high carbon dioxide emitting chemicals that do not significantly contribute to profit. After 2030, emissions cannot continue to decrease without decreases to profit. Every year an investment is made, the slope of the annual profit line changes, reflecting the change in operation regimes as more CCS and CCU is required to maintain policy compliance.

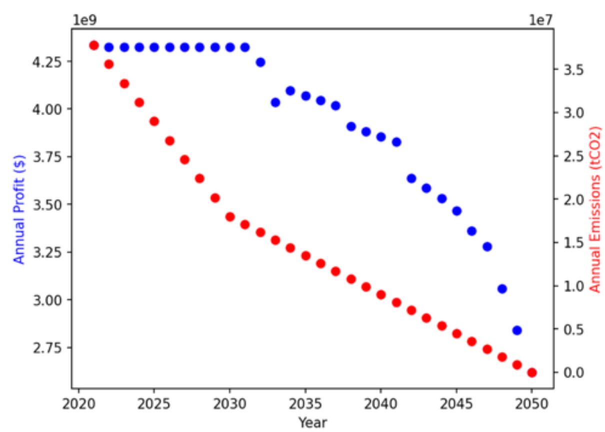

Figure 6. Annual profit and emissions with time for carbon cap policy with reduced CCS and CCU costs

Table 2 displays the investment capacities and capacity expansions for both CCS and CCU technologies under the carbon cap policy. In year 2020, there is a small investment in both CCS and CCU technology during the initial construction of the biorefinery. Initially, annual emissions are reduced by altering operations. In year 2033 and 2047, there is a significant investment in CCU technology. In the year 2041 and 2045, there is an additional investment in CCS technology. There is a higher investment in CCU technology overall due to its lower operating cost, despite its higher capital cost.

Table 2: Initial capacity and expansions for carbon capture technologies under a carbon cap policy

	Carbon Capture Capacity (tCO_2/yr)	
Year	**CCS**	**CCU**
2020	1.9E3	1.1E5
2033	0	5.6E6
2037	0	4.9E6
2041	3.5E6	0
2045	2.1E6	0

CONCLUSIONS

This work formulated a biorefinery process design and capacity expansion problem. A multi-period programming approach was utilized to consider the capacity expansion decisions when carbon pricing increases and carbon caps decrease with time in accordance with benchmarks of the Paris Agreements. The carbon tax, cap-and-trade, and carbon cap policies were formulated as constraints to evaluate their effects on the NPV and EI pareto fronts. The framework allows manufacturers to plan biorefinery product portfolios and future expansion projects considering carbon pricing policies.

The cap-and-trade policy is evaluated to be more profitable compared to the carbon tax policy and includes greater flexibility as a consequence of the purchasing and selling of allowances mechanism as well as the portion of carbon tax free emissions. The carbon cap policy has shown the importance and necessity of reducing the cost of CCUS technologies for chemical plants to adhere to increasingly strict carbon caps over time. The carbon tax policy results in decreased chemical production due to the financial penalty further highlighting the need for low cost CCUS technologies to offset emissions and achieve net zero carbon emissions.

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REFERENCES

1. CO_2 Emissions. Paris: IEA; 2023.
2. Shukla PR, Skea J, Slade R, Al Khourdajie A, Van Diemen R, McCollum D, et al. Climate change 2022: Mitigation of climate change. Contribution of working group III to the sixth assessment report of the Intergovernmental Panel on Climate Change. 2022;10:9781009157926.
3. Yusuf A, Giwa A, Mohammed EO, Mohammed O, Al Hajaj A, Abu-Zahra MR. CO2 utilization from power plant: A comparative techno-economic assessment of soda ash production and scrubbing by monoethanolamine. Journal of Cleaner Production. 2019;237:117760.
4. Wang R, Ashkanani HE, Li B, Morsi BI. TEA of a Unique Two-Pathways Process for Post-Combustion CO2 Capture. Journal of Energy and Power Technology. 2022;4(04).
5. Bank W. State and Trends of Carbon Pricing 2023. Washington, DC: Wolrd Bank; 2023.
6. Luo Y, Ierapetritou M. Multifeedstock and Multiproduct Process Design Using Neural Network Surrogate Flexibility Constraints. Ind Eng Chem Res. 2023;62(5):2067-79.
7. Sabet E, Yazdani B, Kian R, Galanakis K. A strategic and global manufacturing capacity management optimisation model: A Scenario-based multi-stage stochastic programming approach. Omega. 2020;93:102026.
8. Wernet G, Bauer C, Steubing B, Reinhard J, Moreno-Ruiz E, Weidema B. The ecoinvent database version 3 (part I): overview and methodology. Int J Life Cycle Assess. 2016;21(9):1218-30.
9. Huijbregts MAJ, Steinmann ZJN, Elshout PMF, Stam G, Verones F, Vieira M, et al. ReCiPe2016: a harmonised life cycle impact assessment method at midpoint and endpoint level. Int J Life Cycle Assess. 2017;22(2):138-47.