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Multi-objective Design and Optimization for Supply Chain of Modular Methanol Productions

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The integration of renewable energy sources into the methanol production process is recognized as a viable approach to mitigate carbon emissions and promote renewable energy utilization. This study, centered on a modular methanol production system driven by renewable energy, is a multi-objective model encompassing economic and environmental objectives that is established to optimize methanol production sites and supply chain networks under different objectives. In order to balance economic and environmental goals, an optimal compromise point is set, considering both objectives equally important. Results indicate that under the scenario of minimizing total annual costs, the cost is 7.05×10^8 USD. Under the scenario of minimizing total environmental impact, the cost is 7.74×10^8 USD. At the optimal compromise point, the annual total operating cost is 7.07×10^8 USD. The system's environmental impact is equivalent to approximately 1.77×10^5 t of methanol produced by coal gasification technology. In terms of economic objectives, capital costs and electricity expenses during the production process dominate, while the environmental impact is primarily attributed to production processes. The main approach to reducing environmental impact is by altering production site distribution to minimize transportation-related environmental effects.

1. Introduction

Methanol, a pivotal cornerstone of the chemical industry, finds extensive application as both a fuel source and in the fabrication of various commodities (Galan et al., 2023). Recently, several innovative methods for methanol production have emerged. These include synthesizing renewable methanol by combining green hydrogen with carbon dioxide, as well as producing renewable bio-methanol through the utilization of biomass or municipal solid waste. (Roode-Gutzmer et al., 2019). In renewable methanol synthesis systems, the production of green hydrogen relies predominantly on electrolyzing water using renewable energy sources. However, the intermittent nature, variability, and regional disparities in renewable energy availability present significant challenges to its efficient utilization (Qiu et al., 2022). Modular design technology involves standardizing the design and production of essential equipment for the manufacturing process. This approach amalgamates the benefits of economies of scale and economies of quantity to diminish the cost of individual devices. In order to effectively harness renewable energy, modular technology can act as a foundational element, in conjunction with corresponding energy storage systems (Zhang et al., 2019), to enable uninterrupted production driven by renewable energy by facilitating the initiation and cessation of production lines. Based on modular technology, a modular renewable energy-driven carbon dioxide to methanol synthesis system has been developed (Huang et al., 2022), showcasing superior economic benefits compared to large-scale counterparts. Currently, modular technology is predominantly used in the construction of production systems, while its application in supply chains remains unclear. In supply chain studies focused on traditional chemicals, production has largely been oriented towards large-scale operations, with adjustments in capacity primarily achieved through enhancements in production efficiency. Modular small-scale production allows for capacity adjustments directly through line start-ups and shutdowns. To enhance system flexibility, production lines are permitted to adjust capacity within certain limits; however, deviations from rated conditions entail increased costs (Poluzzi et al., 2022). This work proposes a multi-objective model for supply chain design and optimization based on a modular methanol synthesis system, considering variations in renewable energy distribution to meet methanol demand. Unlike traditional

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approaches focusing solely on single objectives, the model integrates economic goals with environmental impacts to evaluate the performance of modular methanol synthesis systems across different objectives. The specific supply chain is shown in Figure 1. The objective function in different scenarios is shown in Eq. (1).

$$\begin{cases} Min\ TAC\left(in\ minimum\ TAC\ scenario\right) \\ Min\ TEI\left(in\ minimum\ TEI\ scenario\right) \\ Max\ \mu^{s\text{-}h}\left(in\ best\ compromise\ scenario\right) \end{cases} \tag{1}$$

Figure 1: Renewable supply chain framework

2. Mathematic model

2.1 Economic objectives

The economic objective function is defined by the Total Annual Cost (TAC), encompassing both capital and operational expenditures, as articulated in Eq. (2).

$$TAC = TCC + TOC \tag{2}$$

2.2 Total capital cost

The total capital costs primarily stem from the construction expenses of modular methanol production lines at various production sites, as delineated in Eqs. (3) to (5).

$$C_p^C = (n_p)^S C_{cs} \tag{3}$$

$$TCC = CRF \sum_p C_p^C Z_p \tag{4}$$

$$CRF = \frac{r(1+r)^f}{(1+r)^f - 1} \tag{5}$$

2.3 Total operating cost

Methanol transportation costs are articulated in Eqs. (6) to (7); electricity consumption costs and initial hydrogen expenses within the methanol production system are delineated in Eqs. (8) to (11); raw material consumption expenses are expressed in Eqs. (12) to (15); the annual total operating cost is represented by Eq. (16).

$$C_{p,d}^{T,MeOH} = F_{p,d}^{MeOH} D_{p,d} P_k \tag{6}$$

$$C^T = \sum_p \sum_d C_{p,d}^{T,MeOH} Z_{p,d} \tag{7}$$

$$C_p^E = n_p^f C_f + n_p^v \left[1 + 1.3 \times \left(1 - \frac{Cap^v}{Cap^f}\right)\right] C_f \tag{8}$$

$$C^E = \sum_p C_p^E Z_p \tag{9}$$

$$C_p^{H_2} = n_p P_{H_2} \tag{10}$$

$$C^{H_2} = \sum_p C_p^{H_2} Z_p \tag{11}$$

$$Dem_p^{CO_2} = Cap_p^{MeOH} \frac{M^{CO_2}}{M^{MeOH} Sel^{CO_2} X^{CO_2}} \tag{12}$$

$$C_p^{R,CO_2} = Dem_p^{CO_2} P_{CO_2} \tag{13}$$

$$C_p^{R,H_2O} = 3 \times Cap_p^{MeOH} P_{H_2O} \frac{M^{H_2O}}{M^{MeOH}\eta} \tag{14}$$

$$C^R = \sum_p (C_p^{R,H_2O} + C_a^{R,CO_2}) Z_p \tag{15}$$

$$TOC = C^T + C^E + C^{H_2} + C^R \tag{16}$$

2.4 Environmental objectives

Employing the Eco-indicator 99 (Goedkoop and Spriensma, 2000) methodology facilitates the quantitative assessment of environmental impacts across the supply chain continuum. The impact of electricity consumption during production is explicated in Eqs. (17)-(18); the impact of methanol products is delineated in Eqs. (19)-(20); the impact of the transportation process is elucidated in Eqs. (21)-(22); the impact of initial hydrogen is outlined in Eqs. (23)-(24); and the total annual environmental impact is succinctly represented in Eq. (25).

$$EI_p^E = \frac{C_p^E}{p_E} e^E \tag{17}$$

$$EI^E = \sum_p EI_p^E Z_p \tag{18}$$

$$EI_p^R = Dem_p^{CO_2} e^{CO_2} + 3 \times Cap_p^{MeOH} \frac{M^{H_2O}}{M^{MeOH}\eta} e^{H_2O} - Cap_p^{MeOH} e^{MeOH} \tag{19}$$

$$EI^R = \sum_p EI_p^R Z_p \tag{20}$$

$$EI_{p,d}^{\mathrm{T}} = F_{p,d}^{MeOH} D_{p,d} e_k^T \tag{21}$$

$$EI^T = \sum_p \sum_d EI_{p,d}^{\mathrm{T}} Z_{p,d} \tag{22}$$

$$EI_p^{H_2} = \frac{C_p^{H_2}}{p_{H_2}} e^{H_2} \tag{23}$$

$$EI^{H_2} = \sum_p EI_p^{H_2} Z_p \tag{24}$$

$$TEI = EI^E + EI^R + EI^T \tag{25}$$

2.5 Mass balance

Quality balance must be maintained between the flow of production and demand.

$$\sum_d F_{p,d}^{\mathrm{MeOH}} = Cap_p^{MeOH} \tag{26}$$

$$\sum_p F_{p,d}^{\mathrm{MeOH}} = Dem_d^{MeOH} \tag{27}$$

2.6 Constraints

The constraints mainly include the limitation of the maximum number of modular methanol production lines in a certain area, as shown in Eqs. (28)-(29), the limitation of modular methanol production lines operating below full load as shown in Eq. (30), the limitation between modular production quantity and capacity as shown in Eqs. (31)-(32), and the limitation between methanol production and demand within the cycle as shown in Eq. (33).

$$\mathrm{MN}_p = round(\frac{PV_p}{\mathrm{E}} - 0.5) \tag{28}$$

$$n_p \le \mathrm{M}N_p \tag{29}$$

$$0.85Cap^f < Cap^v < Cap^f \tag{30}$$

$$n_p = n_p^f + n_p^v \tag{31}$$

$$Cap_p^{MeOH} = n_p^f Cap^f + n_p^v Cap^v \tag{32}$$

$$\sum_p Cap_p^{MeOH} = \sum_d Dem_d^{MeOH} \tag{33}$$

2.7 Tradeoffs between economic and environmental objectives

For multi-objective optimization problems, the multi-objective model needs to be normalized to obtain the optimal result points under different objective weights. In this work, the evaluation function method is adopted for normalization, as shown in Eqs. (34)-(35).

$$\mu_{o-h}^{s-h} = (O_{o-h}^{\max} - O_{o-h}^{s-h}) / (O_{o-h}^{\max} - O_{o-h}^{\min}) \tag{34}$$

$$\mu^{s-h} = \sum_{o-h} \omega_{o-h} \mu_{o-h}^{s-h} \tag{35}$$

3. Case study

This work employs Shandong Province, a prominent hub for methanol consumption in northern China, as a case study. Specifically, the analysis focuses on conventional methanol consumption sectors, including formaldehyde and methanol fuel industries.

3.1 Base parameters

Through computational and statistical methodologies, a comprehensive assessment reveals a total of 16 methanol demand sites. The photovoltaic power generation aggregate across various locales in Shandong Province was derived from statistical analyses (CLOUD, 2023). Factoring in the minimal operational energy constraints inherent to production systems, a discerning process identified 46 prospective sites conducive to methanol production. Three methanol transportation methods have been established, including truck, train, and pipeline. The distances between each production site and its corresponding demand location were obtained on a map. The aforementioned design and optimization model for the multi-objective supply chain of renewable energy-driven modular methanol production is formulated as a mixed-integer nonlinear programming (MINLP) problem. The model comprises 8,188 variables and 6,237 constraints. Solution computations were conducted using GAMS 24.1.3, employing SCIP as the solver for MINLP models, CONOPT for NLP, and CPLEX for MIP.

3.2 The optimal supply chain

The optimal actual supply chain diagrams in different scenarios are shown in Figure 2

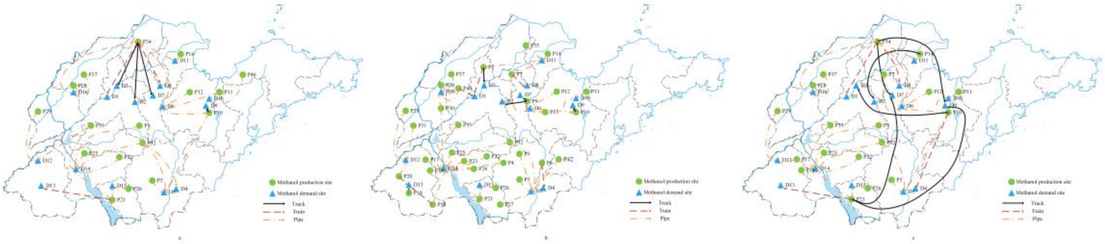

Figure 2: The optimal actual supply chain diagrams in different scenarios. (a Minimum TAC; b Minimum TEI;c Best compromise)

The total annual cost breakdown for different scenarios is presented in Table 1. The total environmental impact for different scenarios is detailed in Table 2. In Table 2, the unit PT is an abbreviation for "point" and represents the result obtained from quantifying environmental impacts using Eco-indicator 99. It represents one-thousandth of the average annual environmental burden per person. The material balance, energy consumption, and methanol cost are shown in Table 3. Considering the selectivity of carbon dioxide and the efficiency of water electrolysis, material imbalances at the inlet and outlet were observed.

Table 1: The total annual cost for different scenarios

Item	Minimum TAC Cost/USD	Minimum TEI Cost/USD	Best compromise Cost/USD
Construction	3.29×10^8	4.00×10^8	3.32×10^8
Initial hydrogen	1.61×10^5	1.61×10^5	1.61×10^5
CO_2	1.13×10^8	1.13×10^8	1.13×10^8
H_2O	4.25×10^6	4.25×10^6	4.25×10^6
Transport cost	7.32×10^6	4.99×10^6	6.48×10^6
Electricity	2.51×10^8	2.51×10^8	2.51×10^8
Total annual cost	7.05×10^8	7.74×10^8	7.07×10^9

Table 2: The total environmental impact for different scenarios

Item	Minimum TAC Impact/PT	Minimum TEI Impact/PT	Best compromise Impact/PT
Methanol product	5.68×10^{7}	5.68×10^{7}	5.68×10^{7}
Production process	1.38×10^{7}	1.38×10^{7}	1.38×10^{7}
Transport Process	5.94×10^{5}	3.98×10^{5}	5.42×10^{5}
Initial hydrogen	2.74×10^{4}	2.74×10^{4}	2.74×10^{4}
Total environmental impact	7.13×10^{7}	7.11×10^{7}	7.12×10^{7}

Table 3: material balance, energy consumption and methanol cost

Item	Item	Item	Methanol cost/USD$\cdot t^{-1}$
Carbon dioxide input/$t\cdot y^{-1}$ 2436667	Electrolyzer/MW 13.1	Minimum TAC case	489.04
Water input/$t\cdot y^{-1}$ 9133300	Compressor/MW 0.479	Minimum TEI case	536.90
Methanol output/$t\cdot y^{-1}$ 1441600	Heater/MW 0.933	Best compromise case	490.43
Waste water output/$t\cdot y^{-1}$ 3054353	Cooler/MW 2.488		
Purge gas output/$t\cdot y^{-1}$ 916306			

In the scenario of minimum TAC, out of 46 regions capable of producing methanol, only 16 are selected for production, indicating a more concentrated methanol production. In the scenario of minimum TEI, 34 are selected for methanol production, indicating a more dispersed methanol production. Compared to the minimum TAC scenario, in this scenario, there are fewer methanol production facilities in each location. This results in a sharp increase in construction costs in each location, and the dispersed distribution of production sites also leads to a decrease in transportation costs. The variation in TEI mainly reflects the reduction in environmental impact caused by transportation. It can be concluded that the main means of reducing TEI in the supply chain model is by changing the distribution of production sites to make them more dispersed, bringing them closer to demand locations, and reducing the environmental impact of methanol commodity transportation to lower the overall system's environmental impact. In the scenario of the best compromise, only 18 regions are selected for methanol production. Compared to the minimum TAC scenario, this scenario includes two additional production sites. It is worth noting that there is a phenomenon of long-distance transportation in this scenario. Because of the low volume, the economic and environmental impact of using long-distance transportation is much lower than if places with large demand switch to more distant supply locations, leading to the phenomenon of long-distance transportation, all of which are routes for methanol transportation by trucks. The environmental impact of the system equates to approximately 1.77×10^{5} t of methanol produced by coal gasification technology, indicating that modular methanol production is more eco-friendly.

4. Conclusions

In this study, a multi-objective model combining economic and environmental goals was proposed based on modular methanol production lines driven by renewable energy sources. The optimal supply chain solutions under different objectives were ultimately obtained. According to the analysis of actual cases, the largest proportion of annual total costs in each scenario is construction costs, while the largest proportion of environmental impact is methanol products. The main way to reduce environmental impact is by altering the distribution of production sites, bringing them closer to demand areas to reduce the environmental impact of transportation. However, this also leads to an increase in construction costs. An optimal compromise point was set, considering economic and environmental goals equally important. At the optimal compromise point, the annual total cost is 7.07×10^{9} USD, and the total environmental impact is 7.12×10^{7} PT.

For supply chain issues, solely considering economic objectives is not comprehensive. In future research, emphasis should be placed on studying the reduction of environmental impact in the methanol production process and developing related multi-period multi-objective models to comprehensively examine the economic benefits and environmental impact of renewable energy-driven modular methanol production lines.

Nomenclature

Variable

C – total construction cost, USD

Cap – capacity, t/y

CRF – the capital recovery factor, /y

Dem – demand, t/y
D – distance, km
E – the energy consumption of a single methanol production line, MW
EI – the total impacts, PT
e – environmental impact per unit consumption, PT/per unit
F – mass flow rate, t/y
f – the operation unit life, -
M – molar mass, g/mol
MN – the maximum number of production lines, -
n – the number of production lines, -
O – solution, -
P – the unit prices of raw material, USD/ per unit
PT – an abbreviation for point, is used to quantify environmental impact, representing one-thousandth of the average annual environmental burden per person, -
PV – photovoltaic power, MW
p – the unit prices, USD/ per unit
r – the interest rate, -
S –the scale up factor, -
Sel – selectivity, -
TAC –total annual cost, USD/y
TCC – total capital cost, USD/y
TEI – the total annual environmental impact, PT
TOC – total operating cost, USD/y
Z – the binary variable, -
μ– the compromise number, -
ω – the weight of objective function, -
Superscript
C – construction
CO_2 – carbon dioxide
E – electricity
f – full-load production line
H_2 – hydrogen
H_2O – water
max – maximum
min – minimum
MeOH – methanol
R – raw material
s-h – the *s-th* solution
T – transportation
v – variable production line
Subscript
CO_2 – carbon dioxide
d – demand site
f – full-load production line
H_2 – hydrogen
H_2O – water
k – mode of transportation
o-h – the *o-th* objective function
p – production site
sc – single modular methanol production line

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