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Techno-economic impacts of using alternative carbon-based feedstocks for the production of methanol

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Abstract

Different alternative carbon sources like CO₂, biomass and plastic waste, can be used to replace fossil carbon as feedstock in the production of methanol. Based on current literature, the plastic-based methanol route is the most competitive one among the three based on price indicator, but there is still a lack of comprehensive understanding of the techno-economic differences between alternative feedstock technologies. In this study, three technologies from each alternative feedstock were assessed to evaluate the techno-economic trade-offs between them. The research shows that even though currently the plastic-based route is comparatively cost competitive with the conventional route of producing methanol, the CO₂-based methanol route can also be competitive with green hydrogen prices in the range of 1400-1100 EUR/t. While the biomass-based route showed superior energy performance compared to the other two.

Keywords: ex-ante technology assessment, alternative carbon-based methanol, comparative process assessment, techno-economic impacts.

1. Introduction

Methanol is a widely used chemical solvent and a chemical building block in the petrochemical industry. It is currently produced at industrial scale using the reforming process of natural gas (methane), at a minimum selling price (MSP) of 300-550 EUR/t. To defossilize the methanol production process, different alternative carbon sources (ACS) like CO₂, biomass and plastic waste are being considered. However, the production processes from ACS are significantly different compared with the conventional process. There have been several techno-economic studies to understand the feasibility of using ACS for the production of methanol. For instance, Sollai et al., (2023) conducted a techno-economic assessment (TEA) for the production of green methanol using captured CO₂ from flue gas and hydrogen from a proton exchange membrane (PEM) water electrolyser (WE). The study showed that a MSP of 960 EUR/t is required to achieve break-even in 20 years for an internal rate of return (IRR) of 8%. Almost 97% of the variable cost and 52% of the bare equipment cost was due to the PEM electrolyser. In the case of biomass-based methanol the price varied according to the technology. For example, de Fournas & Wei, (2022) compared the production of methanol using oxygen gasification of biomass with CO₂ storage and PEM-WE for varying feedstock carbon

utilisation. For the biomass based methanol, they reported that based on the feedstock carbon utilisation, a MSP between 700-1000 EUR/t is required to achieve break-even in 25 years for an IRR of 8%. Afzal et al., (2023) conducted similar TEA on plastic waste to methanol by steam gasification and syngas to methanol process. The research showed that at a MSP of 700 EUR/t, the process achieves a 10% IRR. It also showed that about 58% of the plastic-based methanol MSP was due to the feedstock cost. If we compare these studies, it seems that plastic-based methanol is the most cost competitive. However, because of varying assumptions between such studies, such simple comparisons cannot help to comprehensively assess them against each other. Hence, in this work, we conducted a comprehensive study including technology screening, ex-ante modelling and TEA to compare the techno-economic performance of different ACS feedstocks. The comparison also provides insights into the main hotspots for each route.

2. Methodology

Thirty-two different process routes were identified in literature to produce methanol from ACS feedstocks. To select the most promising technology from each feedstock for ex-ante modelling and TEA, a screening methodology based on the stage-gate concept (section 2.1) was used. The three selected process routes were modelled in Aspen Plus v.12 (section 2.2) and their TEA at process level were calculated using harmonized conditions. The indicators used for the TEA are detailed in section 2.3.

2.1. Technology screening

The screening methodology by Manalal et al., (2023) was applied in this study. It uses different constraints (or gates) to select technologies at each stage; these are technology readiness level (TRL), number of reaction steps, theoretical energy need, carbon utilization efficiency (CUE) and economic constraint (EC) (Manalal et al., 2023). In stage-1, technologies with $TRL > 3$ were selected to the next stage. In stage-2, the ideal stoichiometric reactions of each process route were used and technologies with less than 4 process steps (i.e., stoichiometric reactions) were selected. In stage-3, theoretical heat and electricity requirements were estimated through the standard enthalpy change (ΔH^0) and Gibbs energy change (ΔG^0). At this stage, using the ideal stoichiometric reactions, the CUE of each process route was also calculated using Eq. (1). Based on the needed energy and CUE, the different process routes were ranked.

$$\text{Carbon utilisation efficiency (CUE)} = \frac{\text{Moles of carbon atom in product}}{\text{Moles of carbon atom in feedstock}} \quad (1)$$

Processes with an electricity need below 750 kJ/mol methanol and a CUE =100% were selected from each feedstock to the next stage. In stage-4, EC was calculated using Eq. (2) and chemical prices adjusted to 2018 base year.

$$\begin{aligned} \text{Economic constraint (EC)} \\ = \frac{\sum_{\text{reactants}} \text{mass flow} * \text{Component price} + (\Delta H^0 \text{ or } \Delta G^0)_{\text{endergonic}} * \text{Utility price}}{\sum_{\text{products}} \text{mass flow} * \text{Component price}} \end{aligned} \quad (2)$$

Technologies with $EC < 1$ were selected in stage-4. In stage-5, the technologies were ranked based on TRL, number of process steps and EC; only one process route for each feedstock was selected.

2.2. Ex-ante modelling

The methanol production capacity of each of the three selected technologies was 400 kt/y, as it corresponds to the total methanol demand in the port of Rotterdam, with a purity >

99 wt%. The three selected technologies modelled in Aspen Plus were: CO₂ direct hydrogenation to methanol (C2M), biomass steam gasification (BSG) with syngas to methanol (S2M) and, plastic steam gasification (PSG) with S2M. Green hydrogen from WE was considered as hydrogen feedstock source in all three cases. The C2M process was modelled following the work by E. Lücking & de Jong, (2017), using an RPlug reactor with kinetic input data. The BSG process was modelled as per the GoBiGas Project in Sweden (Larsson et al., 2018), with the gasification section modelled as a combination of an RStoic (gasification & char formation section) and RGibbs reactors (tar formation section). After gasification, a Rectisol process and cryogenic distillation were used for syngas cleaning. The P2G process was modelled as per Quevedo et al. (Quevedo et al., 2021), combining an RStoic and an RGibbs reactor. The methanol synthesis section (S2M) in both, biomass and plastic-based routes, was modelled based on the work by E. Lücking & de Jong, (2017).

Four different steam levels were used as heating utilities, namely: low low pressure (LLP at 3.9 bar), low pressure (LP at 5.5 bar), medium pressure (MP at 21 bar) & high pressure (HP at 51 bar) steams. To supply heating needs at a temperature above 250 °C when the process could not provide them, combustion-based heat was provided and natural gas (81.4 wt% CH₄, 14.4 wt% N₂, 3 wt% C₂H₆, 1 wt% CO₂, 0.2 wt% C₃H₈) was used as utility. Cooling water (25 °C to 40 °C), chilled water (propylene glycol mixture) and refrigerants (R134a, R1150 & R50) were used as cooling utilities. Electricity was the only non-thermal utility defined in the simulation models. The models considered process heat integration, maximising the internal use of heat.

2.3. Techno-economic assessment

The indicators used to compare the three processes were: CUE of the process (Eq. (1)), energy requirements, MSP, capital expenditure (CAPEX) and operational expenditure (OPEX). A sensitivity analysis by varying the electricity price was conducted to understand the impact of hydrogen price on MSP. The CAPEX was calculated based on working capital, inside battery limit (ISBL), outside battery limit (OSBL), engineering (EN) and contingency (CN) costs with estimates from Towler & Sinnott, (2013), as shown in Table 1. The bare equipment (BE) cost for ISBL cost calculations were obtained from Aspen Economic Analyzer. The OPEX calculation was based on variable and fixed OPEX with estimates also from Towler & Sinnott, (2013), as shown in Table 1.

Table 1: Assumptions for economic calculations (Towler & Sinnott, 2013).

CAPEX		Fixed OPEX	
ISBL cost	3.3*BE	Maintenance cost	3%*ISBL
OSBL cost	40%*SBL	Capital charges & royalties	4%*(ISBL+OSBL+EN)
Engineering costs	10%* (ISBL+OSBL)	Labour, supervision & overhead cost	1.875*Labour estimates
Contingency	10%* (ISBL+OSBL)	Corporate income tax (CIT)	25%*Operating income
Working capital	5%*(ISBL+OSBL+EN+ CN)	Land & building rents, insurance, property taxes & environmental charges	5%*(ISBL+ OSBL)

Variable OPEX such as raw materials, utilities and wastewater treatment costs were calculated based on mass flows, obtained from Aspen, and prices. The revenue was calculated from products and excess utilities, and using a payback period of 12 years, the MSP of methanol was calculated. In this study, it was assumed that only the methanol price varied and the other product prices remained unchanged, among the lifetime of the

plant (i.e., 25 years). The economic calculations were based on 2018 as the base year and Netherlands as the plant location.

3. Results and discussion

3.1. Technology screening

From the literature, 11, 15 and 6 possible 3-step routes were identified to synthesise methanol from CO₂, biomass and plastic waste, respectively. Regarding H₂ feedstock, electrochemical-based technologies were crucial for CO₂ routes, while due to the inherent hydrogen content in biomass and plastic molecules; electrochemical, biochemical and thermal routes were possible. The three selected technologies for further assessment were:

Table 2: Selected technologies for each ACS and their corresponding screening values.

Technology	Reaction steps	Electricity	Heat	CUE	EC
WE + C2M	2	712 kJ/mol	-93 kJ/mol	100%	0.89
BSG + WE + S2M	3	237 kJ/mol	-19 kJ/mol	100%	0.39
PSG + S2M	2	0 kJ/mol	112 kJ/mol	100%	0.34

Note: WE- Water electrolysis, C2M- CO₂ to methanol, BSG- Biomass steam gasification, S2M- Syngas to methanol, PSG- Plastic steam gasification

3.2. Ex-ante modelling and techno-economic assessment

A comparative assessment of mass flows for the selected technologies shows that the CO₂ and plastic-based methanol routes have a higher CUE. Moreover, the CO₂-based route showed least technical complexity in terms of number of process streams and temperature range. The biomass-based route showed the lowest CUE and the highest process complexity. This is due to a higher range of waste and by-product streams, as shown in Table 3.

Table 3: Mass flow comparison of the selected technologies for each ACS vs base-case natural gas for the synthesis of methanol.

Parameter		Base case fossil methanol	CO ₂ to methanol	Biomass to methanol	Plastic waste to methanol
Feedstock	Carbon feedstock	330 kt (natural gas)	800 kt (CO ₂)	860 kt (biomass)	310 kt (plastic waste)
	Water	899 kt	981 kt	881 kt	220 kt
Products	Methanol	405 kt	406 kt	411 kt	408 kt
	Oxygen	-	871 kt	334 kt	-
	Methane	-	-	44 kt	-
Waste	Wastewater	614 kt	240 kt	670 kt	5 kt
	Purge	198 kt	248 kt	70 kt	34 kt
	Off gases	12 kt	16 kt	48 kt	8 kt
	Char & ash	-	-	143 kt	13 kt
	Tar	-	-	21 kt	62 kt
Process CUE		80%	69%	49%	68%

Two differences can be observed between CO₂ and biomass-based routes. First is the significant amount of oxygen produced compared to other routes. The second difference regards to the hydrogen requirement. As the biomass-based route produces hydrogen during steam gasification, only part of the total amount of hydrogen required for methanol production was provided by WE, while in the CO₂-based route the hydrogen is fully provided by WE. For the plastic-based route, no external hydrogen was needed as all the required hydrogen was produced during the plastic steam gasification process.

Table 4: Energy flow comparison of the selected technologies for each ACS vs base-case natural gas for the synthesis of methanol. (Note: A negative sign means generation.)

Main utilities	Base case fossil methanol	CO ₂ to methanol	Biomass to methanol	Plastic waste to methanol
Electricity	198 GWh/y	7168 GWh/y	3553 GWh/y	220 GWh/y
LLP steam	-385 TJ/y	-76 TJ/y	-89 TJ/y	-
LP steam	259 TJ/y	-1895 TJ/y	-1899 TJ/y	1792 TJ/y
MP steam	-1085 TJ/y	-269 TJ/y	-1127 TJ/y	-1389 TJ/y
HP steam	-36 TJ/y	-	-3203 TJ/y	-615 TJ/y
Natural gas	2635 TJ/y	-	-	2509 TJ/y
Cooling water	3894 TJ/y	6209 TJ/y	10543 TJ/y	2565 TJ/y

Table 4 highlights that the need and/or production of utilities are significantly different between the different ACS routes. Thus, changing from conventional methanol production to ACS routes, can affect other interlinked utility providers or users in an existing industrial cluster thereby leading to potential cascading impacts. In terms of steam generation, the biomass-based routes outperformed the other two.

Table 5: Economic comparison of the selected technologies for each ACS vs base-case natural gas for the synthesis of methanol.

Economic indicators	Base case fossil methanol	CO ₂ to methanol	Biomass to methanol	Plastic waste to methanol
Methanol MSP (EUR/t)	520	1950	1390	860
CAPEX* (MEUR)	358	432	957	403
OPEX (MEUR/y)	171	746	495	309

*H₂ is considered as raw material & cost is included in OPEX

The economic assessment showed that none of the alternative routes is competitive at the moment with the fossil-based route. The plastic-based methanol could be produced at the lowest MSP (860 EUR/t) compared to biomass (1390 EUR/t) and CO₂ (1950 EUR/t) based methanol. For the biomass-based route, the higher price was due to the higher capital expenditure on the biomass gasification and syngas cleaning steps. For the CO₂-based route, the higher price was due to the high operational expenditure affected by the high price of green hydrogen (4000-6000 EUR/t). A sensitivity analysis to understand the impact of the price of green hydrogen on these technologies was conducted by varying the electricity price used for green hydrogen production and it is shown in Figure 1.

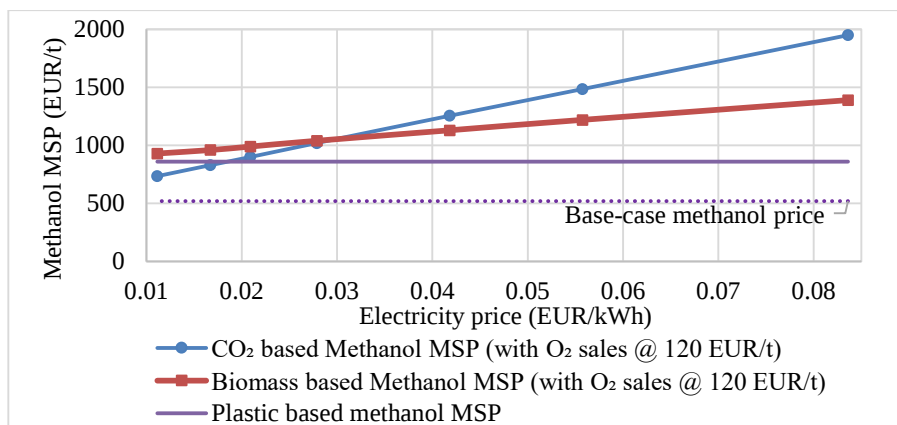


Figure 1: Impact of electricity price on CO₂, biomass & plastic based methanol prices.

The analysis shows that at a green hydrogen price of 1400-1100 EUR/t, the CO₂ route can be cost-competitive. For instance, at a green hydrogen price of 1350 EUR/t, CO₂ route had an MSP of 735 EUR/t, compared to the biomass route (930 EUR/t) and the plastic route (860 EUR/t).

4. Conclusions

This paper indicates that plastic waste gasification to produce methanol currently performs technically and economically better than CO₂ and biomass-based synthesis routes. The work also shows that the CO₂ hydrogenation-based route can potentially become competitive in a scenario with renewable electricity prices below 0.02 EUR/kWh, outperforming biomass & plastic gasification-based methanol. The bio-based route can be competitive when demand of heat/steam along with methanol is critical.

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