

Techno-Economic Assessment of Decarbonization Pathways for Methanol and Formaldehyde Production: A Superstructure Optimization Approach

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ABSTRACT

This study aims to compare different pathways for achieving CO₂ emission reductions during the production of methanol and, subsequently, formaldehyde, i.e., its major derivative. An equation-oriented model of the formaldehyde sector is developed, incorporating a superstructure of various transition pathways including feedstock switching (biomass, biogas, waste), process electrification (Power-to-X), and CO₂ capture. The OSMOSE tool is used to evaluate the superstructure and compare the alternative production pathways on the basis of thermodynamic, environmental, and economic key performance indicators for future scenarios (2025 and 2050). Furthermore, to cope with the limitations of predefined pricing scenarios, a parameter sweep is performed, exploring a broader set of economic conditions and seeking to identify the zones of economic optimality associated with each configuration through the solving of a Mixed-Integer Linear Programming cost minimization problem, while generalizing the analysis results beyond a specific year or geographic context. Finally, the potential of industrial symbiosis implementation, between clinker and formaldehyde production facilities, as a cost-reduction measure for Power-to-X processes is assessed.

Keywords: Formaldehyde, Methanol, Energy Transition, Technoeconomic Analysis, Superstructure Optimization, Industrial Symbiosis

INTRODUCTION

The chemical industry is an energy-intensive and highly-emitting sector, representing 6.5% of the global greenhouse gases emissions [1]. Methanol (MeOH) is a key building block for solvents, plastics, and fuels. Its major application is its conversion to formaldehyde which accounted for 23% of global MeOH demand in 2023 [2]. Formaldehyde, of chemical composition CH₂O, is an organic chemical used as a raw material for the production of resins, polyurethanes, paints and coatings, pharmaceuticals, food intermediates, and chelating agents. It is produced from MeOH via two main routes: the silver process and the metal oxide process [3]. In the silver process, operated at high temperature (580–680°C) and under air deficiency, MeOH is converted into formaldehyde through catalytic dehydration ($\text{CH}_3\text{OH} \rightleftharpoons \text{CH}_2\text{O} + \text{H}_2$) using a silver-based catalyst. On the other hand, the metal oxide process consists of a direct catalytic MeOH oxidation ($\text{CH}_3\text{OH} + 0.5 \text{O}_2 \rightarrow \text{CH}_2\text{O} + \text{H}_2\text{O}$), performed over a

metal oxide catalyst (e.g. iron, molybdenum, or vanadium oxide). The reaction is implemented at medium temperatures (270–430°C) and in the presence of excess air, enabling very high MeOH conversion around 99%. Although European formaldehyde production in 2017 was almost evenly split between the silver and metal oxide processes, this study focuses on the latter given that recent investments tend to favor the metal oxide route [3].

Direct process emissions during formaldehyde production, stemming from MeOH or formaldehyde over-oxidation, are negligible [3]. The environmental impact of formaldehyde is thus closely linked to the carbon footprint of MeOH feedstock. However, current methanol production is almost entirely fossil-based. Indeed, MeOH is predominately produced from natural gas with steam methane reforming (SMR, ~65%) or coal gasification (~35%, mainly in China), while biomass and other renewable feedstocks account for less than 1% of global production [4]. This results in a high carbon footprint ranging from 0.8 up to more than 4 t CO₂/t MeOH produced [5].

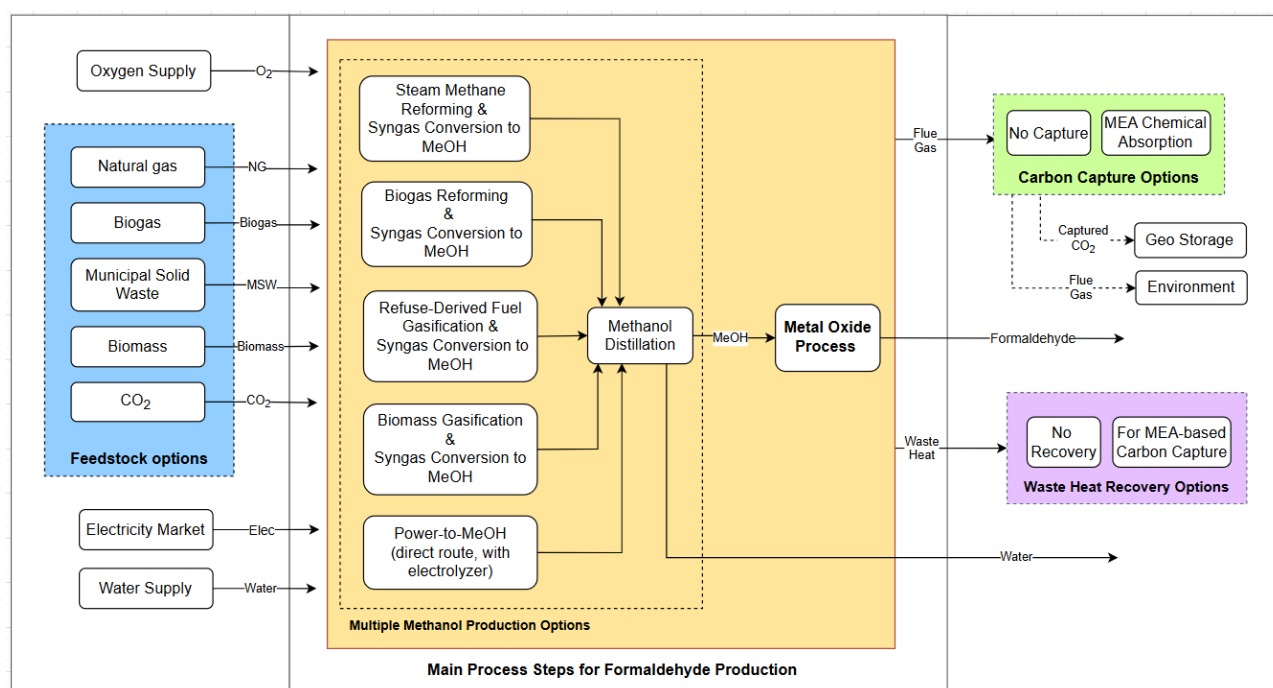


Figure 1. Superstructure for formaldehyde industry.

Hence, decarbonizing MeOH production through biomass use, CO₂ capture (CC), and process electrification [6] is essential for reducing the environmental impact of the European chemical sector.

METHODOLOGY

This study aims to compare various pathways for achieving CO₂ emission reduction during the production of methanol and, subsequently, formaldehyde, i.e. its major derivative. The methodological framework is adopted from our previous study [7]. Thorough literature review and data collection, from academic papers, institutional reports, and Best Available Techniques reference document [3], are first carried out, aiming at gathering information on the production process under study and applicable emission mitigation pathways. These pathways include energy efficiency improvement, feedstock switching, process electrification, and CO₂ capture and storage.

The collected data are used to develop an equation-oriented model of the formaldehyde sector, written in Lua language, consisting of mass and energy balances, as well as economic considerations such as annualized investment (CAPEX) and operating (OPEX) costs. This model incorporates a superstructure (depicted in **Figure 1**) of various MeOH production routes, including synthesis from syngas generated via (1) conventional Steam Methane Reforming (base case, NG), (2) biomass gasification (BM), (3) biogas tri-reforming (BG), (4) refuse-derived fuel (RDF, from municipal solid waste (MSW)) gasification, as well as (5) power-to-MeOH (P2X) process

converting CO₂ and hydrogen (H₂, produced by alkaline electrolysis) into e-methanol. CO₂ in flue gases, from MeOH or formaldehyde production, may be emitted to the environment or captured through monoethanolamine (MEA)-based chemical absorption, using waste heat from the metal oxide process. Configurations abbreviations, process descriptions, and modeling details can be found in the Supplementary Sections **S1** and **S2**.

The production routes previously mentioned are compared based on different key performance indicators (KPIs) including specific energy demand (GJ/t CH₂O), CO₂ emissions (t CO₂/t CH₂O), and total cost (€/t CH₂O). Specific energy demand encompasses fuel and electricity requirements for an easier comparison across configurations. Specific total emissions include direct and indirect emissions. Direct, or scope 1, CO₂ emissions stem from product/feedstock over-oxidation or fuel combustion during formaldehyde or MeOH production. Biogenic CO₂ does not contribute to scope 1 emissions, while captured biogenic CO₂ is accounted as negative emission. Indirect emissions arise from feedstock supply and electricity production. CO₂ emission factors are listed in the Supplementary Section **S3**. Finally, the specific total cost (STC) encompasses both annualized CAPEX (for a green-field scenario) and OPEX considerations including feedstock, fuel, electricity, CO₂ emission (no free allowances or revenues for negative emissions), as well as transport and storage (T&S) of captured CO₂.

The OSMOSE tool, developed by the IPESE group of EPFL [8], is used to evaluate the superstructure and a Mixed-Integer Linear Programming (MILP) problem is

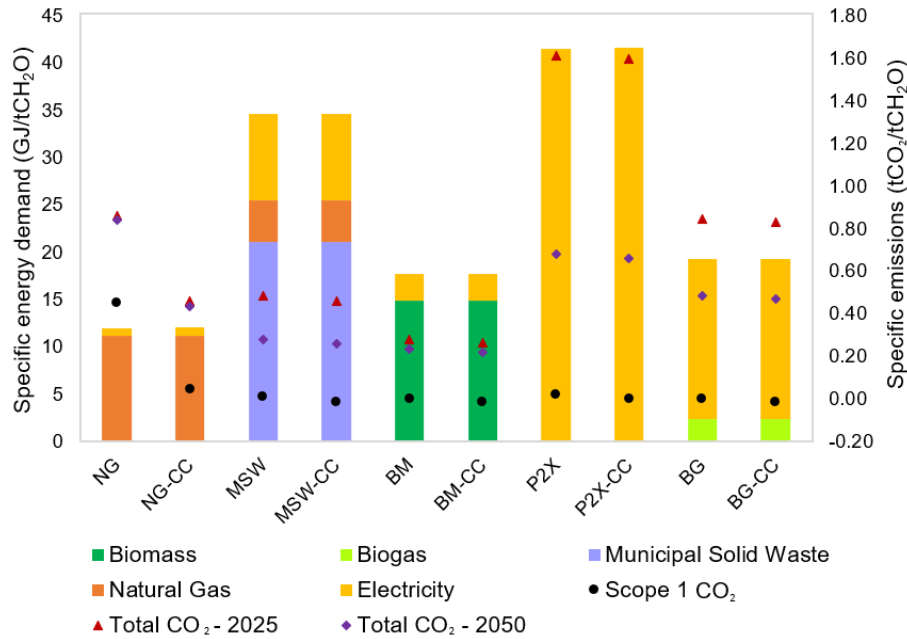


Figure 2. Specific energy demand (left axis) and scope 1 and total CO₂ emissions (right axis) in 2025 (electricity is sourced from the current Belgian grid) and 2050 (electricity is supplied by the 2050 European electricity mix) scenarios for different production routes.

solved to identify the optimal decarbonization configurations for two different energy and emissions scenarios: (1) the 2025 scenario, considering current energy and CO₂ prices in Belgium, and (2) the 2050 scenario, based on estimated future marginal production costs, considering higher ETS and lower energy prices [9-13]. Economic data for both scenarios are listed in **Table 1**.

Table 1: Economic parameters considered for 2025 and 2050 scenarios.

Scenario	2025	2050
Electricity (€/MWh)	78	58
Natural gas (€/MWh)	36	40
Biomass (€/MWh)	17	18
Biogas (€/MWh)	40	30
MSW (€/MWh)	9	9
ETS (€/tCO ₂)	80	200
CO ₂ T&S (€/tCO ₂)	50	50
CO ₂ supply (€/tCO ₂)	80	80

The high volatility of energy prices—stemming from changing global political landscape, availability limitations, and regulatory shifts—prevents the accurate identification of future optimal production routes. To cope with the limitations of predefined pricing scenarios, a parameter sweep is performed, exploring a broader set of economic conditions and seeking to identify the zones of economic optimality associated with each configuration, while generalizing the analysis results beyond a specific

year or geographic context. The price of natural gas (p_{NG}), electricity (p_E), municipal solid waste (p_{MSW}), biomass (p_{BM}), biogas (p_{BG}), and CO₂ supply (p_{CO2}), as well as the ETS price (p_{ETS}) are varied within the pricing sets specified in **Table 2**. For each of the 30, 000 resulting combinations, MILP optimization is performed, seeking total cost minimization. The results are analyzed to identify robust decarbonization pathways.

Table 2: Pricing sets considered for the parameter sweep.

Parameter	Set of values
p_{NG}	[10, 25, 50, 75, 100] €/MWh
p_E	[10, 25, 50, 75, 100] €/MWh
p_{MSW}	[-5, 0, 5] €/MWh
p_{BM}	[10, 25, 50, 75, 100] €/MWh
p_{BG}	[10, 25, 50, 75, 100] €/MWh
p_{CO2}	[0, 25, 75, 100] €/t
p_{ETS}	[75, 100, 200, 300] €/t

RESULTS

Energy demand and CO₂ emissions reduction

From **Figure 2**, total energy requirement (including fuel and electricity, and excluding feedstock) of conventional formaldehyde production (NG) amounts to 11.96 GJ/t CH₂O. Feedstock switching options result in higher total energy requirements: +61% for BG and +248% for

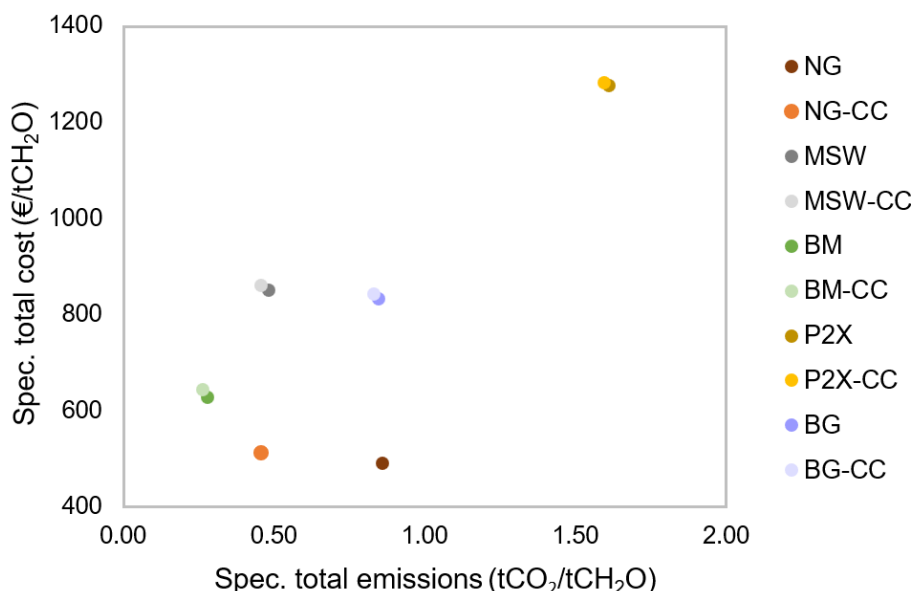


Figure 3. Specific total cost (€/t CH₂O) vs. total CO₂ emissions (t CO₂/t CH₂O) – 2025 scenario.

P2X due to H₂ production via alkaline electrolysis; +48% for BM and +189% for MSW due to lower process efficiency (e.g., drying requirements, lower carbon conversion) and additional energy requirements during MSW pre-treatment. Direct CO₂ emissions from formaldehyde production (i.e., 0.018 t CO₂/t CH₂O generated by over-oxidation) or fossil CO₂ emitted by MeOH production can be captured through chemical absorption with MEA. Heat integration between formaldehyde production and CC unit completely covers the additional heat demand and reduces the energy penalty of CO₂ capture to 0.01–1.1% compared to counterparts without CC.

While feedstock switching decreases drastically scope 1 CO₂ emissions (96–100%) compared to NG (0.452 t CO₂/t CH₂O), the contribution of indirect emissions, stemming from upstream material extraction and electricity production, results in a shift in trends as can be seen in **Figure 2**. Total CO₂ emissions breakdown can be found in Supplementary Material (Figure S3).

Based on current emission factors in Belgium (2025 scenario), BG and P2X routes are associated with total emissions, respectively, only 1% lower and 88% higher than NG due to large electric demand. The least emitting options are BM-CC (-69%) and BM (-68%), followed by NG-CC and MSW-CC (-47%). On the other hand, clear environmental advantage appears for feedstock switching options when low-carbon electricity (e.g., from the projected 2050 European electricity grid) is considered. Carbon footprint reduction between 45% and 77% can be achieved with alternative feedstocks, making NG-CC less environmentally competitive (-49% compared to base case), while P2X corresponds to a modest emission mitigation of 23%. While a 47–49% reduction in CO₂

emissions can be achieved by implementing CC in natural gas-based facilities, capturing CO₂ from electrified, bio-, and waste-based processes represents little interest in terms of carbon footprint (1–3% additional reduction) since only a limited amount of CO₂, stemming from formaldehyde production, is treated.

Scenario-based economic assessment

Economics being an important decision variable for industrial energy transition, scenario-based economic assessments are depicted in **Figure 3** and **Figure 5**. Despite the environmental benefit of alternative feedstocks, the economically optimal configuration in the 2025 scenario is NG (€489/t CH₂O), closely followed by NG-CC, reducing total CO₂ emissions by 47% and increasing STC only by 5%. High specific CAPEX (204–399% increase compared to NG for P2X and BM-CC respectively, as can be seen in **Figure 4**), low CO₂ ETS price, and expensive electricity (€78/MWh_e vs. €36/MWh_{NG}) result in alternative production pathways being economically uncompetitive compared to fossil-based chemicals. Indeed, configurations relying on MSW achieve similar environmental performance as NG-CC with a 67% higher cost. The current Belgian electricity mix results in P2X configurations being the least attractive, both from an economic and environmental perspective. On the other hand, BM and BM-CC achieve drastic emission mitigation (68–69%) at a reasonable cost (+28–32% compared to NG).

In the 2050 scenario, relying on lower energy costs and higher ETS price, NG-CC reduces the STC by 9% compared to the base case (€553/t CH₂O). Access to decarbonized electricity improves the environmental ranking of electricity-intensive configurations such as MSW,

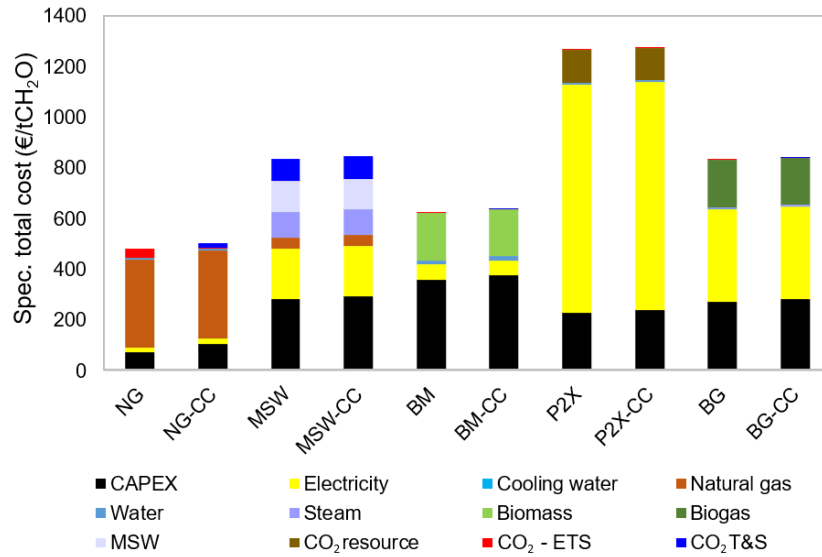


Figure 4. : Specific total cost breakdown – 2025 scenario.

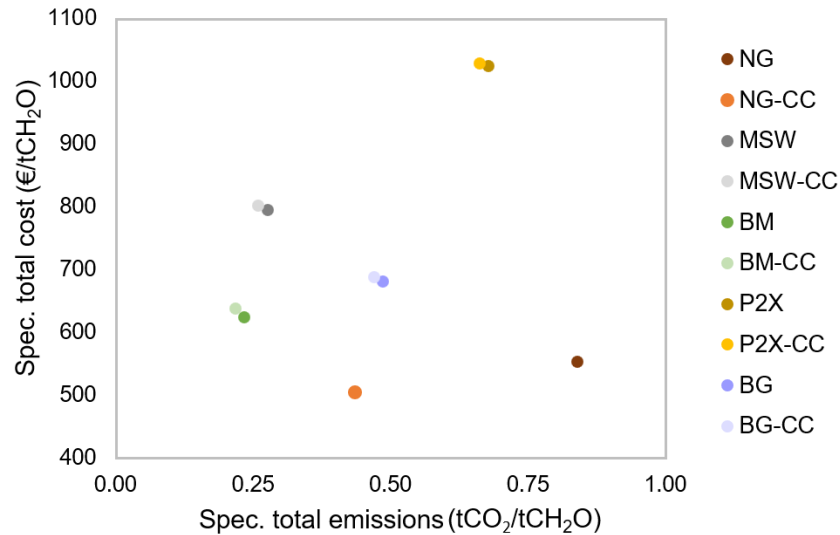


Figure 5. Specific total cost (€/t CH₂O) vs. total CO₂ emissions (t CO₂/t CH₂O) – 2050 scenario.

BG, and P2X. Biogas-based options benefit from cheaper electricity, reducing the cost gap with the base case down to only 23%, while production pathways relying on MSW are still 44% more expensive than NG. Despite lower emissions, formaldehyde produced from e-methanol feedstock remains the most expensive option with STC exceeding €1,000/tCH₂O. Formaldehyde production from biomass represents the most promising non-fossil-based route, with a 13–15% increase in STC and 73–75% of emission reduction compared to NG.

Parameter sweep

The ranking of production pathways previously presented is valid solely for the commodities prices considered for the analysis. To cope with the high uncertainty of future energy and feedstock prices, a parameter

sweep is performed, exploring a broad set of economic conditions. For each price combination, the configuration achieving the lowest production cost is identified. The results of the parameter sweep are represented in parallel coordinates plots (see **Figure 6** and Supplementary Section **S5**), enabling the identification of robust and flexible solutions for decarbonized formaldehyde production. As a general comment, CC implementation is favored over counterparts without CC for high ETS prices ($\geq$ €200/t CO₂). Moreover, as can be seen in **Figure 6**, natural gas price is a key parameter driving technology selection.

According to the performed analysis, SMR is the technology with the highest number of occurrences (14,744), followed by biogas reforming (4,884), MSW gasification (4,837), and power-to-X (4,071), while biomass gasification was found to be optimal only in 1,464 times

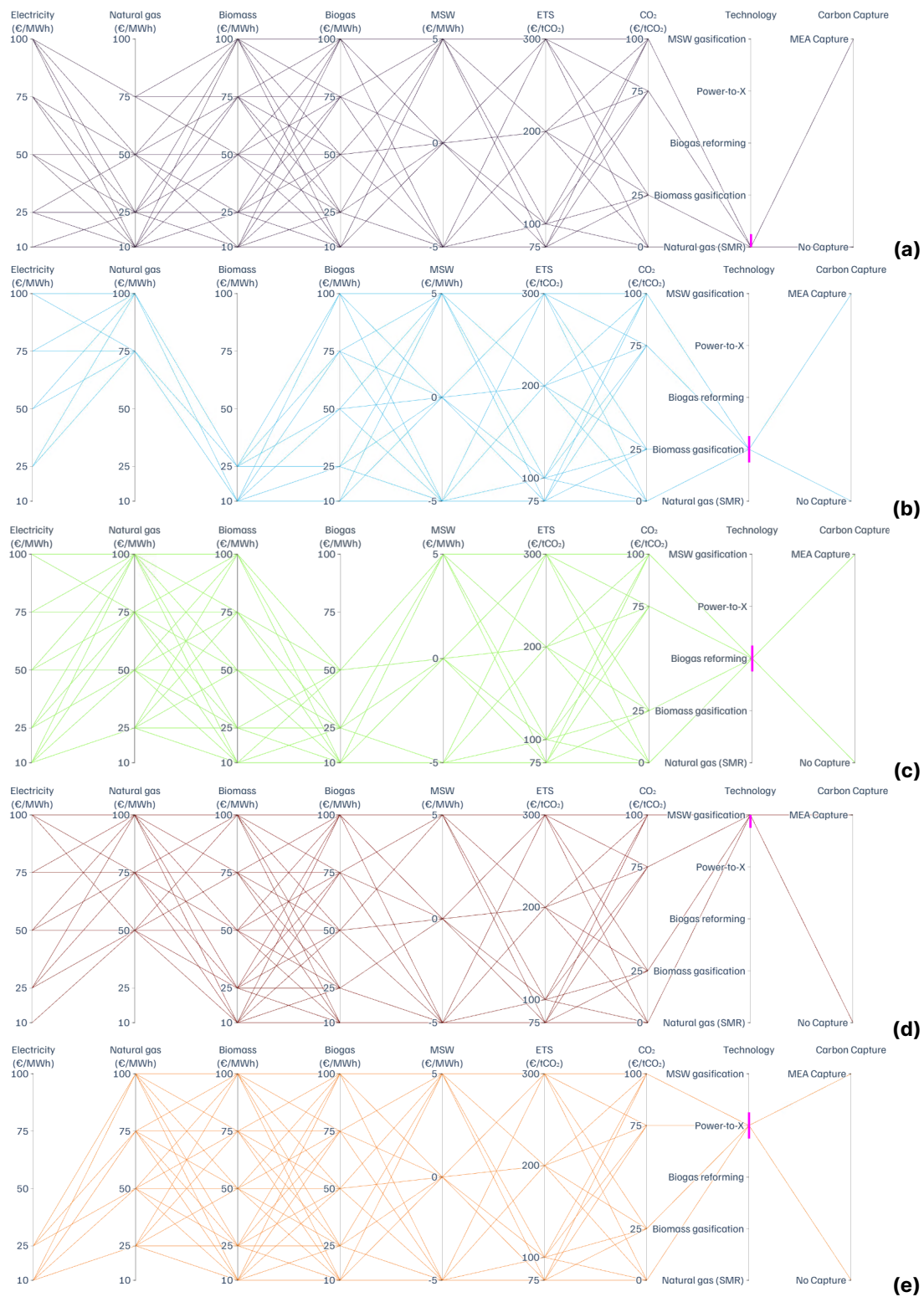


Figure 6: Solution space of economic optimality for (a) natural gas-, (b) biomass-, (c) biogas-, (d) MSW-based, and (e) electrified formaldehyde production routes.

out of 30,000 scenarios tested.

Natural gas-based (**Figure 6a**) routes are identified as optimal for a wide range of economic conditions,

making it a flexible and robust solution from an economic point of view. On the other hand, for BM and BM-CC (**Figure 6b**) to appear as economically optimal solutions,

market conditions must combine cheap biomass ($\leq \text{€}25/\text{MWh}$) and expensive natural gas ($\geq \text{€}75/\text{MWh}$). Moreover, electricity price should not be in the lower bracket ($\geq \text{€}25/\text{MWh}$ for a biomass price of $\text{€}10/\text{MWh}$; $\geq \text{€}75/\text{MWh}$ when biomass is available at $\text{€}25/\text{MWh}$) to avoid favoring electricity-intensive configurations.

Biogas-based options (Figure 6c), which offer greater flexibility than biomass-dependent alternatives, become economically viable when natural gas prices exceed $\text{€}25/\text{MWh}$ and $\text{€}50/\text{MWh}$ for, respectively, BG-CC and BG. These options may remain optimal even at higher biogas prices ($\text{€}50/\text{MWh}$), provided that electricity prices are low to moderate ($\text{€}25\text{--}50/\text{MWh}$).

Economic optimality for P2X and P2XCC (Figure 6e) requires extremely cheap electricity ($\leq \text{€}25/\text{MWh}$) combined with natural gas and biogas available at a higher price. Moreover, the lower the MSW price, the lower the CO_2 supply price should be to remain competitive with MSW-based options. On the contrary of other technologies, P2X-CC is always favored over P2X except when low ETS price ($\text{€}75/\text{tCO}_2$) is combined with free CO_2 feedstock.

Finally, a negative MSW price alone is not sufficient to ensure the economic optimality of MSW and MSW-CC configurations (Figure 6d). The availability of natural gas at a sufficiently high price ($\geq \text{€}50/\text{MWh}$) is required.

As a conclusion, the parameter sweep revealed that NG and NG-CC are the most flexible and robust production pathways. This highlights the challenge of transitioning the chemical sector away from fossil feedstocks. However, biogas and waste-based technologies arise as interesting candidates for non-fossil MeOH and formaldehyde production.

Potential of industrial symbiosis for the production of e-chemicals

As previously mentioned, bio-based options arise as interesting candidates from an environmental and economic perspective for the energy transition in the chemical sector. However, availability issues are to be expected due to heavy reliance on biomass for industrial decarbonization [14]. Hence, to completely phase out chemicals production from fossil fuels, power-to-X processes should be included to some extent in the production mix. Nonetheless, the economic assessment reveals that e-MeOH feedstock represents the least cost-effective decarbonization pathway for formaldehyde production in a wide range of scenarios.

To address elevated costs, the potential of industrial symbiosis (IS) as a cost-reduction measure is investigated. IS [15] is a systemic approach that promotes collaboration among industries by resources exchanges, such as energy, water, and by-products, enhancing collective sustainability of industrial processes. In the present study, synergies between a formaldehyde

production plant ($0.1 \text{ Mt CH}_2\text{O}/\text{y}$) and nearby cement industry ($0.9 \text{ Mt clinker}/\text{y}$) are considered. Commodities prices assumed for this analysis are listed in Table 3.

Table 3 : Economic parameters for IS implementation.

Commodities	Cost	
Coal	11.5	€/MWh
Municipal Solid Waste	3	€/MWh
Electricity	58	€/MWh
CO_2 ETS	200	€/t CO_2
CO_2 T&S	50	€/t CO_2

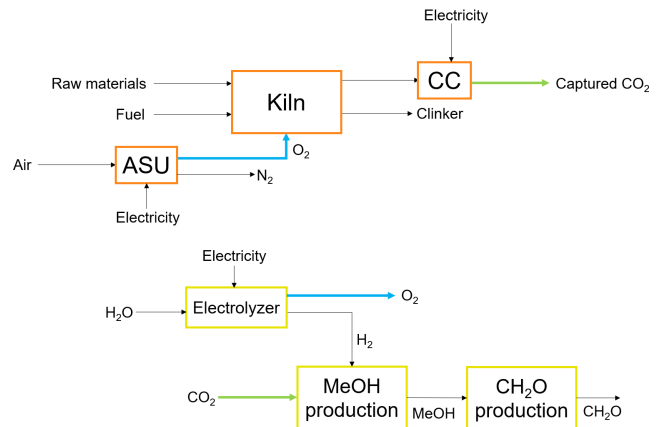


Figure 7. Case study for IS implementation between cement and formaldehyde industries.

The base case configuration of the system is depicted in Figure 7. In our previous study [16], oxy-fired kiln with cryogenic CO_2 capture arises as one of the most promising decarbonization options for the cement industry and hence is chosen as the production route for the IS case. In this configuration, heat is provided by burning a mixture of MSW and coal in oxygen produced by an Air Separation Unit (ASU). The generated CO_2 is subsequently captured via a cryogenic capture unit, before being transported and stored. On the other hand, the formaldehyde facility generates oxygen as a by-product of water electrolysis, which is necessary for hydrogen production. Meanwhile, CO_2 is required as a feedstock for MeOH production.

Competitiveness of clinker production and power-to-X process can be improved by mutualizing CO_2 capture unit and electrolyzer costs through CO_2 and oxygen exchanges, as highlighted in Figure 7. Such synergies result in an ASU that is no longer necessary, as the oxygen generated by the electrolyzer ($0.17 \text{ Mt O}_2/\text{y}$) entirely covers the oxygen demand of the cement kiln ($0.12 \text{ Mt O}_2/\text{y}$). Furthermore, the cement plant provides the entire CO_2 feedstock for methanol production ($0.16 \text{ Mt CO}_2/\text{y}$), reducing the amount of CO_2 that needs to be transported and stored ($0.59 \text{ Mt CO}_2/\text{y}$ vs. $0.75 \text{ Mt CO}_2/\text{y}$ without IS).

Removing the ASU from the system reduces total

electricity demand by 2% (-28 GWh_e/y), which represents 4.2 kt CO₂/y considering the current carbon intensity of Belgian electricity. Regarding the economics of the system, instead of buying CO₂ from the market at the ETS price (€200/t CO₂, representing the maximum marginal abatement cost industries are willing to bear, as well as the long-term target cost of CO₂ supplied by Direct Air Capture (DAC)), the formaldehyde facility is supplied by the cement plant at a much lower cost (i.e., capture cost of €27/t CO₂). Moreover, oxygen sales to the cement plant result in annual economies of about €11.5M. Despite the use of expensive oxygen (€91/t O₂ when produced via electrolysis vs. €30/t O₂ when produced with ASU), the cement plant benefits from CO₂ sales (€4.3M/y). Moreover, the reduced amount of CO₂ to be transported and stored represents additional economies of €8M/y. The implemented synergies and corresponding economies achieved are schematically represented in **Figure 8**.

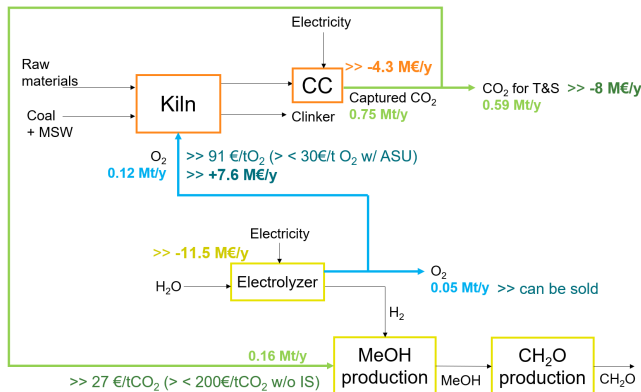


Figure 8. Synergies and corresponding economies achieved by IS implementation.

Hence, the implementation of synergies between these industries reduces the total production cost by 3% and by 32% for clinker and formaldehyde, respectively, compared to estimations without IS. Despite the decreased production cost in the IS case, P2X formaldehyde remains more expensive than other decarbonization options such as NG-CC and bio-based routes. Therefore, this option only makes economic sense when there is a scarcity of biomass, high natural gas prices, or low electricity prices. These conditions make P2X options difficult to appear as competitive decarbonization pathways for formaldehyde production.

Table 4: Specific total cost of clinker and formaldehyde with and without implementation of IS.

	No symbiosis	With symbiosis	
Clinker	121	118	-3%
(€/t _{clinker})			
Formaldehyde	1207	815	-32%
(€/t _{CH2O})			

Total (M€/y)	229.8	187.5	-18%
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CONCLUSION

This study provides a foundation for decision-making regarding CO₂ emission mitigation for formaldehyde production based on thermodynamic, environmental, and economic KPIs for future scenarios. For this purpose, an equation-oriented superstructure of formaldehyde industry was developed, encompassing various energy transition pathways including feedstock switching (biomass, biogas, waste), process electrification (Power-to-X), and CO₂ capture.

Despite requiring more energy (+ 48–247%) than the base case (11.96 GJ/tCH₂O), alternative feedstocks result in reductions of total CO₂ emissions up to 77% when low-carbon electricity is used, while emissions are cut by almost half when CC is implemented at NG-based facilities.

The economic assessment in the 2025 scenario identified NG as the most interesting configuration from an economic perspective, closely followed by NG-CC (5% cost increase, 47% emissions reduction compared to base case). Conversely, expensive and fossil-based electricity results in P2X being both the most expensive and most emitting configuration. The most promising bio-based options are BM and BM-CC: 28–32% cost increase, 65–67% emissions reduction compared to NG. If lower energy prices and higher ETS price are assumed (2050 scenario), NG-CC becomes the most cost-effective option, followed by biomass-based configurations, while electrification (P2X) remains the most expensive production route.

A parameter sweep, exploring a broad set of energy pricing scenarios, was also performed. An MILP problem was solved with the OSMOSE tool for each price combination to identify the solution space in which each configuration is associated with the lowest specific total cost. From the 30, 000 pricing scenarios tested, NG-based options (NG and NG-CC) were found to be the most flexible and robust production pathways, representing 49% of the optimal solutions identified. NG-CC exhibits reasonably good environmental performance, with emissions cuts reaching nearly half of current levels, despite its continued reliance on fossil fuels. The most interesting bio-based route is biogas reforming, appearing as optimal as long as moderate-to-high natural gas prices are combined with low-to-moderate electricity prices. On the contrary, stringent conditions for economic optimality arise for BM and P2X configurations requiring extremely low biomass and electricity prices respectively (≤25€/MWh).

Finally, the potential of industrial symbiosis as a cost-reduction measure for power-to-X process was assessed. Synergies between oxy-fired clinker production (requiring oxygen and capturing CO₂) and formaldehyde

production from e-MeOH (generating oxygen by electrolysis and requiring CO₂ as feedstock) result in reduced electricity demand (-2%) and reduced production costs (-3% for clinker and -32% for formaldehyde). However, P2X formaldehyde remains more expensive than other emission mitigation options, only making economic sense when biomass scarcity, high natural gas prices, and low electricity prices are observed.

These observations highlight the difficulty for the chemical sector to decarbonize and the importance of process efficiency improvements as well as policy frameworks and governmental funding to ensure competitiveness of low-carbon formaldehyde production routes.

DIGITAL SUPPLEMENTARY MATERIAL

Process descriptions, modeling details, and additional results can be accessed here: LAPSE:2026.0027

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