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Evaluation of centralized/decentralized configuration schemes of CO2 electrochemical reduction-based supply chains

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Abstract

Electrochemical reduction of CO_2 (CO_2ER) is an emerging technology with the potential to limit the use of fossil-based feedstocks in the petrochemical industry by converting CO_2 and renewable electricity into useful products such as syngas. Its successful deployment will depend not only on the technology's performance but also on its integration into the supply chain. In this work, a facility location model is used to gain insights regarding the capacity of CO_2ER plants that produce syngas and the implications for the central/decentral placement of these CO_2-based syngas plants. Different optimal configurations are examined in the model by changing the syngas transport costs. In this exploratory case, the results indicate that centralization is only an option when the syngas and CO_2 transport costs are similar. When syngas transport is more expensive, decentralizing CO_2-based syngas plants in the supply chain appears more feasible.

Keywords: CO_2 electrochemical reduction; CO_2 utilization, supply chain modeling, optimization, supply chain configurations

1. Introduction

The European Green Deal includes the 2030 Climate Target Plan targeting a greenhouse gas (GHG) emission reduction of at least 55% in 2030 compared to 1990 levels and a net-zero GHG emissions target by 2050 (European Commission, 2019). This requires a drastic change in the petrochemical industry, which is challenging due to the industry's dependence on fossil fuels as its carbon feedstock. Currently, processes using CO_2 as an alternative feedstock are being developed. In the electrochemical reduction of CO_2 (CO_2ER), CO_2, water, and electricity are converted into a range of intermediates and final products that can be used for further chemical and fuel synthesis in multiple sectors. CO_2ER is not yet a mature technology, and ultimately it will be integrated into already existing supply chains (SCs), which affects the SC configurations in terms of implementation scale and (de)centralization of the technology. In order to study the impact of the CO_2ER technology in connection with its SC, a facility location optimization model was developed in the current work to understand the potential trade-offs of decentralized/centralized configurations when replacing fossil-based syngas with CO_2-based syngas from a CO_2ER process. Centralized/decentralized business cases for CO_2ER are explored from an SC perspective in the European petrochemical context using a hypothetical case study. Syngas is chosen as the product of interest, as it is a large-scale fossil-based industrial product, commercialized as a versatile commodity that can be used as a precursor for a wide range of processes in the petrochemical industry (Choe et al., 2022; Ebbehøj, 2015). Syngas is a mixture of hydrogen and carbon monoxide (CO). The CO molecule in syngas makes the mixture toxic, which adds safety requirements to the transportation and handling of this feedstock. Alternative feedstocks for syngas production are described in SC literature; the primary focus has so far been on the upstream part of the SC (e.g., (Ahmadvand and Sowlati, 2022; Marufuzzaman et al., 2016)). In these studies, the current business model is employed where syngas is produced on-site (i.e., without storage and transport). Transporting syngas to establish a centralized market is not considered. This work investigates how an industrial scale CO_2-based syngas SC could look like for different syngas transportation costs in relation to CO_2 transport costs. The facility location model selects the optimal locations, the number of CO_2-based syngas plants, the plant capacities, and connections between echelons in a three-stage SC, see Figure 1A.

2. Mathematical model formulation of CO2-based syngas supply chain

A fixed charge facility location problem (FLP) is formulated as a mixed integer linear program (MILP). This model is an uncapacitated multiple allocation FLP; the maximum size of the CO_2-based syngas plant is not constrained, and individual echelons can connect to multiple other echelons. The problem is formulated as a p-median problem, the foundations of which are laid by Hakimi (1964). The model is based on the SiLCaRD (simultaneous location of central and regional distribution facilities) model formulated in the work of Götzinger (2013).

Mass balance constraints ensure that the amount of CO_2 captured in the system is in equilibrium with the amount of syngas at the demand locations and that mass conservation is guaranteed. Location constraints specify where to establish and open the CO_2-based syngas plants, while allocation constraints select and connect the different echelons in the system. The piecewise linear transport constraints allow for dealing with non-linearities in transport. The mathematical is elaborated below and the decision variables are emphasized in bold font:

H	set of CO_2 source locations, indexed by *h*
J	set of potential CO_2-based syngas plant locations, indexed by *j*
K	set of syngas demand locations, indexed by *k*
Q	set of transport segments of the piecewise linear cost function, indexed by *q*
A_q	slope [$€_{2020}$/kilometer/Mtonne transported] of segment *q* in the piecewise linear transport cost function
B_q	intercept [$€_{2020}$] of segment *q* in the piecewise linear transport cost function
C_{hj}	distance [kilometers] from CO_2 source *h* to CO_2-based syngas plant *j*
C_{jk}	distance [kilometers] from CO_2-based syngas plant *j* to syngas consumer *k*
CC_h	average carbon capture cost [$€_{2020}$/Mtonne] at the CO_2 source (at cluster level)
CF_{st}	cost factor of syngas transport [$€_{2020}$ syngas transported /$€_{2020}$ CO_2 transported]
SG_{Conf}	CO_2-to-syngas conversion factor [Mtonne syngas/Mtonne CO_2]
$\boldsymbol{yq_{hj}}$	1 if the CO_2-based syngas plant *j* is assigned to CO_2 source *h* in segment *q* of the piecewise linear transport function, 0 if not
$\boldsymbol{yq_{jk}}$	1 if the syngas consumer *k* is assigned to the CO_2-based syngas plant *j* in segment *q* of the piecewise linear transport function, 0 if not
$\boldsymbol{z_{hjq}}$	size [in Mtonne of CO_2 transported] from CO_2 source *h* to CO_2-based syngas plant *j* in segment *q* of a piecewise linear function
$\boldsymbol{z_{jkq}}$	size [in Mtonne syngas] transported from CO_2-based syngas plant *j* to syngas consumer *k* in segment *q* of a piecewise linear function

The objective function aims to minimize the yearly capture costs at the industrial cluster (1a), the yearly pipeline transport cost of CO_2 from CO_2 sources to CO_2-based syngas plants (1b), and the yearly (hypothetical) pipeline transport cost of syngas from CO_2-based syngas plants to syngas consumers (1c). The amount of CO_2 captured (z_{hjq}) and the size of the electrolyzer (z_{jkq}) is determined as a result of the minimization of the objective function to fulfill the syngas demand in the SC. A piecewise linear transport cost function is applied to all the transport links between the echelons in the model. The amount of CO_2 (from source to CO_2-based syngas plant) is multiplied with a CO_2-to-syngas conversion factor to calculate the plant's syngas production; see equation (2).
Objective function - minimize:

$$\underbrace{\sum_{h\in H}\sum_{j\in J}\sum_{q\in Q} z_{hjq} * CC_h}_{(1a)} + \underbrace{\sum_{h\in H}\sum_{j\in J}\sum_{q\in Q} A_q * z_{hjq} * C_{hj} + B_q * yq_{hj}}_{(1b)} + \underbrace{\sum_{j\in J}\sum_{k\in K}\sum_{q\in Q} (A_q * z_{jkq} * C_{jk} + B_q * yq_{jk}) * CF_{st}}_{(1c)}$$

$$SG_{Conf} * \sum_{h\in H}\sum_{q\in Q} z_{hjq} = \sum_{j\in j}\sum_{q\in Q} z_{jkq} \qquad \forall\, j \in J \qquad (2)$$

3. Case study – CO_2-based syngas supply chains

A B

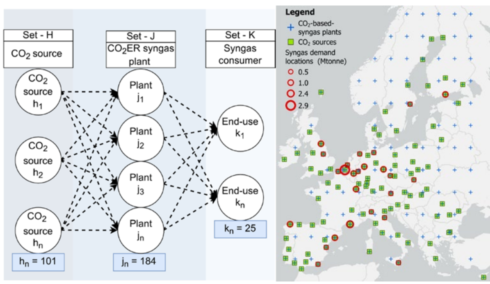

Figure 1 - A – Representation of the three-echelon supply chain model described in this case study. B – Industrial CO_2 sources in Europe, potential CO_2 -based syngas plant locations, and syngas demand locations with sizes.

The model uses geographical data from industrial clusters in Europe (EU-27+UK). It uses a discrete grid of potential CO_2-based syngas plant locations. A 100 x 100 grid was placed to create potential location sites for CO_2ER plants from the borders of Portugal to Finland. For the purpose of this study, plant locations over the sea were disregarded, and the industrial cluster locations were added as potential location sites, resulting in 185 potential electrolyzer locations, see Figure 1B. The current case study contains CO_2 emission data from 101 industrial clusters (with 944 individual plants within these clusters from 9 types of industries: ammonia, cement, lime, iron & steel, refining, petrochemical, oil & gas, power generation, and aluminum). Industry-specific CO_2 impurities were not considered, and it was assumed that CO_2 is in the same conditions irrespective of its source. The dataset is available via ArcGIS online (Boston Consulting Group, 2021) and is based on the European Pollutant Release and Transfer Register (European Environment Agency, 2020). The following considerations were taken into account:

• The worldwide syngas market was 150 Mtonne in 2018 (Jouny et al., 2018), with a CAGR of 9.5% it is estimated to reach 180 Mtonne in reference year 2020 (Inkwood Research, 2017). Europe uses approximately 22% of global syngas, with 51% in the petrochemical industry (IMARC, 2021). The estimated syngas demand in Europe's petrochemical industry used in this work was 20.3 Mtonne/year. In the model, the demand needs to be assigned to specific locations. In order to assign different syngas demands to different (hypothetical) sites, a syngas plant size of 0.482 Mtonne/year was assumed based on the syngas demand of a standard methanol plant size of 0.4 Mtonne/year (Ebbehøj, 2015). To fulfill the syngas demand using this standardized size, 42 CO_2-based syngas plants would be necessary. 42 of the 84 petrochemical plants in the European dataset were randomly selected to serve as syngas demand locations. The demand was summed when the selected plants were part of the same cluster.

• The costs of CO_2 transport were based on (hypothetical) existing onshore pipelines (i.e., only operating costs are considered). A piecewise linearization is used based on the values by d'Amore (2021).

• This work assumes an existing syngas transportation infrastructure (i.e., only operating costs are considered). Currently, there is limited data available on the transportation of syngas. Direct use of syngas is the dominant business case causing the lack of existence of commercial-scale syngas transportation networks. The costs of syngas transport are therefore highly uncertain and likely more expensive than CO_2 transport due to additional safety requirements. For the latter, Knoope (2015) has shown how CO_2 transport costs increase with additional safety measures. In this study, the costs of syngas transport are based on the transport costs of CO_2 but were multiplied with different cost factors to investigate its effect on the centralized/decentralized deployment and the SC configuration.

• The capture costs of CO_2 were averaged at the cluster level based on the mass of CO_2 emissions of individual plants in that cluster and the capture costs per industry. These capture costs [in $€_{2020}$] were based on the capture cost from Global CCS Institute (2021) and CO_2 compression costs from IEA (2020). The CO_2 coming from the petrochemical, oil, and gas industries was assumed to have the same capture and compression cost as from the oil refining industry.

4. Case study results

The problem formulation was formulated in GAMS (41.1) and optimized using the CPLEX 22.1.0.0 MIP solver. The system ran with an Intel®Core™ i7-1185G7 CPU 3GHz processor and 32GB RAM. The problem comprised 228,893 variables, of which 93,526 were binary and 350,303 equations. The model was solved for five different transport cost factors (CF) values (1-3) and took 11 minutes.

The SC configurations with varying cost factors for syngas transport are presented in Figure 2, while the different SC characteristics are presented in Table 1. For all the CFs, the same 25 syngas demand locations were selected. Plants were co-located when the CO_2 source, the CO_2-based syngas plant, and the syngas consumer were within the same industrial cluster. Co-locating reduces transport dependency; however, in some cases, CO_2/syngas transport was still needed to fulfill the syngas demand or desired to optimize costs. Remote CO_2 capture and transport can be cheaper to (partly) fulfill the demand compared to on-site capture due to capture cost differences between clusters. When the transport of syngas was more expensive than CO_2 co-locating the CO_2 source with the CO_2-based syngas plant became more viable. In CF2.5, there remains a need for CO_2 transport to 5 clusters to fulfill syngas demand. The cost factors affect the capacity of the

Table 1 Supply chains characteristics for different syngas transport cost factors

Cost factor	Capacity CO_2-based syngas plants			CO_2 sources	CO_2-based syngas plants	Co-located plants
[-]	[Mtonne syngas]			[#]	[#]	[#]
	Min	Max	Avg.			
1	0.24	3.5	0.99	21	21	15
1.5	0.24	3.5	0.87	24	24	18
2	0.24	3.5	0.87	25	24	20
2.5	0.50	3.0	0.83	26	25	21
3	0.50	3.0	0.83	26	25	21

individual plants, as the average capacity is higher at a lower cost factor. In other words, lower transport cost increase plant capacity leading to a more centralized SC.

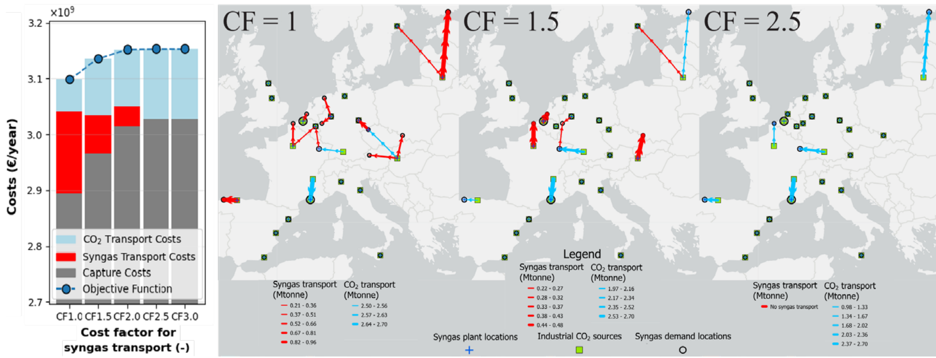

Figure 2 - Parts of the objective function for different syngas transportation costs factors and CO_2-based syngas supply chains with different syngas cost factors.

The total SC cost in the objective function is hardly affected by an increase in syngas transportation cost, see Figure 2. The CF1 SC can benefit from the cheapest CO_2 capture sources. When syngas transport becomes more expensive, the model chooses to pay more for capturing CO_2 at less favorable locations to avoid transportation. At a CF of 2.5, syngas transport is eliminated.

5. Conclusion and future work

A simplified CO_2-based syngas supply chain facility location model was developed in this work. The objective minimized the CO_2 capture, transportation, and syngas transport costs. In this case, when syngas transportation has the same price as CO_2 transport, there are options for centralization in the CO_2-based syngas SC. At higher syngas transportation costs, decentral SCs are preferred. When syngas transport is as expensive as CO_2 transport, syngas transport is favored due to its lower transport volume and potential to capitalize on clusters with lower capture costs. CO_2 transport is occasionally necessary for clusters with insufficient CO_2 to fulfill their syngas demand after CO_2ER conversion.

In the next iteration of the model, a sensitivity analysis will be performed by exploring different syngas demand locations and sizes, which will help generalize the findings of this specific case. The current model is a starting point for developing a more exhaustive CO_2-to-syngas-based SC model, focusing on enhancing transportation details and refining the objective function. With this exploratory case, the first insights were gained regarding the scale of CO_2-based syngas plants and the preference for a centralized/decentralized configuration of the SC.

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