



# Optimizing the Design of Supply Chains for Carbon Capture, Utilization, and Sequestration in Europe: A Preliminary Assessment

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Carbon capture and storage represents a key technology for reducing the anthropogenic emissions of greenhouse gases. In addition to this, carbon utilization has often been considered as a viable option for increasing the environmental benefits, while decreasing costs of the mere capture and storage system. This contribution proposes an optimization framework for the design of carbon capture, transport, utilization, and storage supply chains in the European context. Based on literature data, technologies converting CO<sub>2</sub> into methanol and polyether carbonate polyols were selected as the most promising and incorporated into the optimization framework. The goal is to reduce 50% of European emissions from large stationary sources by 2030. Results highlight that, under our assumptions, the significance of carbon utilization in terms of a reduction of the environmental impact is likely to be a minor one: considering the current state of technologies only about 2.4% of the overall CO<sub>2</sub> emitted from large stationary sources can be removed by chemical utilization. However, significant benefits can be obtained in terms of overall cost reduction thanks to revenues deriving from the chemicals being produced.

**Keywords:** carbon capture utilization and storage, supply chain optimization, mixed integer linear programming, European framework, CO<sub>2</sub> chemical conversion and utilization

## 1. INTRODUCTION

The anthropogenic generation of greenhouse gases (GHGs) has led to an increment of the average surface temperature, with dramatic consequences for the natural environment. The target of limiting the rise in average temperature to +1.5°C by 2050 was indicated (IPCC, 2018). In the European Union (EU), in order to comply with the Paris Agreement, it has been proposed to reduce GHGs and particularly CO<sub>2</sub> emissions by 43% by 2030 with respect to 2005 values. Carbon capture and storage (CCS) technologies represent a promising candidate for attaining sustainable development (Li et al., 2019), i.e., an economic growth that aims at tackling major environmental issues (global warming), in an era when power and industry still massively rely on carbon and, more in general, fossil fuels.

Overall, CCS is employed to dispose the CO<sub>2</sub> emitted by the operation of carbon intensive facilities into appropriate geological basins (CCS), in opposition to the possibility of converting it into useful products (CCU), or exploiting a combination of both sequestration and utilization (CCUS). The typical CCS scheme is composed of three echelons: capture, transport, and sequestration (IPCC, 2005). Three main technologies are currently available for capturing CO<sub>2</sub>

from the use of fossil fuels: post-combustion capture, oxy-fuel combustion capture, and pre-combustion capture (Bui et al., 2018). The concentrated CO<sub>2</sub> flow is then purified and compressed to be transported in a cost-effective way. Finally, the third step is the injection of CO<sub>2</sub> below the Earth's surface and its consequent sequestration. As an alternative to geological sequestration into appropriate basins, CO<sub>2</sub> could be diverted for the use of processes traditionally fed by fossil fuels, with the aim of producing commodities while pursuing a negative carbon footprint (Smit et al., 2014). Regarding utilization pathways, different options have been highlighted as promising in attaining a reduction of the costs of CCS through either CCU or CCUS, and have been gathered into groups of mineral carbonation, chemical conversion, and biological utilization (US National Academy of Sciences, 2019). Several studies have considered the technological feasibility of different routes, among which chemical conversion has emerged as the most appropriate option (at least in techno-economic terms) for an early-stage implementation of CCU (Lehtonen et al., 2019). For instance, Alper and Yuksel Orhan (2017) recently reviewed the possible chemical conversion options for CO<sub>2</sub> and from their analysis a broad variety of families of both pathways and products, attractive for CCUS, emerged (e.g., C1-chemicals, catalytic processes, polymers, inorganics, fine chemicals). Sternberg et al. (2017) analyzed the CO<sub>2</sub>-based production of some C1-chemicals by assessing the potential benefits in terms of lowering global warming and fossil depletion; Barbera et al. (2020) assessed the technical performance of conversion paths into C1-chemicals. Armstrong and Styring (2015) highlighted the environmental benefits achievable in treating CO<sub>2</sub> as a commodity chemical rather than a waste product. On the other hand, other studies questioned the actual effectiveness of the chemical conversion of CO<sub>2</sub> and indicated that only minor environmental benefits could be obtained (Mac Dowell et al., 2017).

Recently, a noteworthy research effort has laid the foundations for several studies on CCS and CCUS, which have provided a large increase in the techno-economic knowledge of each single stage of the supply chain (SC). Moreover, the necessity of investigating the design, cost, and integration of the CCS/CCUS stages for different geographic contexts and applicative frameworks has emerged (Bui et al., 2018). Several contributions analyzed, mostly through mixed integer linear programming (MILP) techniques, the design and optimization of CCS systems for different geographic contexts and scales (**Table 1**). Han and Lee (2012) optimized a CCS SC for North Korea through a MILP formulation under uncertainty in market prices while, again for North Korea, a subsequent contribution considered preference on risk as a measure of data uncertainty (Lee et al., 2017). Middleton et al. (2012) proposed a MILP model for CCS located in Texas that also took into account uncertainty in storage physics. Again, the response toward uncertainty in storage physics was investigated by Middleton and Yaw (2018) for the case of a CCS SC in Alberta, Canada. Another MILP CCS optimization was published for the United Kingdom by Elahi et al. (2014), which has subsequently been updated by also including uncertainty in carbon prices (Elahi et al., 2017).

Again, for the United Kingdom, another MILP optimization under uncertainty in market prices and subsidies was developed by Nie et al. (2017). Similarly, Kalyanarengan Ravi et al. (2016) proposed a CCS SC modeling framework for the context of the Netherlands. d'Amore and Bezzo (2017) optimized a European CCS SC, also considering the risk of leakage related to the pipeline transport (d'Amore et al., 2018), and aspects of social acceptance and risk perception (d'Amore et al., 2020). Zhang et al. (2018) proposed a theoretical MILP modeling tool for the optimization of CCS systems under both storage physics and cost uncertainties.

The first model on CCUS SC optimization was proposed by Turk et al. (1987) and included the possibility of employing CO<sub>2</sub> for enhanced oil recovery (EOR) in Ohio (United States). Klok et al. (2010) adopted a similar approach for an infrastructure located in Norway. Hasan et al. (2015) in their US-wise optimization framework took again into account EOR as the only possible utilization option. A theoretical modeling framework for EOR was proposed by Wu et al. (2015), too. Ağrali et al. (2018) proposed an optimization model for CCUS located in Turkey, where again, only EOR was adopted as a carbon utilization sink. An even more limited number of scientific contributions optimize CCUS systems by considering the conversion and utilization of CO<sub>2</sub> to generate valuable products. For South Korea, Han and Lee (2013) and Lee et al. (2019) considered the conversion of CO<sub>2</sub> into either biobutanol or green polymers as an alternative to geological storage within a comprehensive CCUS modeling framework. For Germany Leonzio et al. (2019) optimized a CCUS SC through a MILP modeling tool that included the possibility to produce methanol as an alternative to geological storage. Finally, Kim et al. (2019) produced a MILP formulation for the integration of a hydrogen/CCUS SC in the context of South Korea.

Overall, considering the framework of modeling, simulation, and optimization of CO<sub>2</sub> SCs, very few contributions optimized comprehensive CCUS superstructures (i.e., continent-wide) and, in particular, most of these considered only EOR as a unique utilization pathway, given its well-known practice and capability of generating profits. However, although there is great potential with EOR, it is not recognized as a viable and large-scale solution in Europe (Geske et al., 2015). On the other hand, those very few articles including other routes (such as methanol, bio-butanol, and polymers) are focused on a regional-to-countrywide level, and never address the problem of CO<sub>2</sub> conversion and utilization at the European scale. This contribution aims at filling this gap by proposing a large-scale European CCUS SC optimization, with the main goal of addressing the echelon of CO<sub>2</sub> conversion into useful products through a tailored design stage. Regarding the possible CO<sub>2</sub> conversion options, major research issues remain open and need to be tackled, such as scalability and costs, especially for mineral carbonation and biological pathways (US National Academy of Sciences, 2019). This study will only take into account chemical conversion as a potential utilization route, in opposition to the mere geological sequestration into appropriate basins. The resulting MILP modeling tool will provide insights into the optimal design of comprehensive CCUS systems at a noteworthy geographic scale, to provide researchers,

**TABLE 1** | Literature review on published contributions on SC optimization for CCS/CCUS.

References	CC(U)S	Utilization	Scale (Area)	Uncertainty
Turk et al. (1987)	CCUS	EOR	Region (Ohio, United States)	–
Klokk et al. (2010)	CCUS	EOR	Country (Norway)	–
Han and Lee (2012)	CCS	–	Region (Pohang, South Korea)	Prices, costs
Middleton et al. (2012)	CCS	–	Region (Texas, United States)	Storage physics
Han and Lee (2013)	CCUS	Biobutanol, polymers	Region (Pohang, South Korea)	Prices, costs
Elahi et al. (2014)	CCS	–	Country (United Kingdom)	–
Hasan et al. (2015)	CCUS	EOR	Country (United States)	–
Wu et al. (2015)	CCUS	EOR	Region (theoretical)	Inexact parameters
Kalyanarengan Ravi et al. (2016)	CCS	–	Country (the Netherlands)	–
d'Amore and Bezzo (2017)	CCS	–	Continent (Europe)	–
Elahi et al. (2017)	CCS	–	Country (United Kingdom)	Carbon prices
Lee et al. (2017)	CCS	–	Region (Pohang, South Korea)	Preference on risk
Nie et al. (2017)	CCS	–	Country (United Kingdom)	Market, subsidies
Ağrali et al. (2018)	CCUS	EOR	Country (Turkey)	–
d'Amore et al. (2018)	CCS	–	Continent (Europe)	–
Middleton and Yaw (2018)	CCS	–	Region (Alberta, Canada)	Storage physics
Zhang et al. (2018)	CCS	–	Region (theoretical)	Storage physics, costs
d'Amore et al. (2019)	CCS	–	Continent (Europe)	Storage capacity
Lee et al. (2019)	CCUS	Biobutanol, polymers	Region (Pohang, South Korea)	Preference on risk
Leonzio et al. (2019)	CCUS	Methanol	Country (Germany)	–
Kim et al. (2019)	CCUS	Hydrogen	Country (South Korea)	–
d'Amore et al. (2020)	CCS	–	Continent (Europe)	–
d'Amore and Bezzo (2020)	CCS	–	Continent (Europe)	–

investors, and policy makers with a methodological framework for quantitative and strategic analysis of a range of possible alternatives for a significant decrease in European CO<sub>2</sub> emissions.

The article is organized as follows. The modeling framework and its main assumptions will be characterized within the next section, after which the description of the MILP model will follow. Further input parameters and the complete mathematical formulation are reported in the **Supplementary Material**. Subsequently, the case studies and results will be presented, and the main limitations of the study will be critically analyzed and discussed. Some final remarks will conclude the work.

## 2. MODELING FRAMEWORK

This contribution proposes a MILP model for the economic optimization of European CCUS SCs. Although based on a time-static architecture (to reduce the computational burden), the model is conceived to capture a fixed quota of the CO<sub>2</sub> emissions that it is forecasted to be produced from large-stationary sources throughout the next decade (i.e., from 2020 to 2030). In particular, the SC takes into account (**Figure 1**):

- the location and emission of large stationary sources of CO<sub>2</sub> in Europe, according to data provided by the EDGAR Database (JRC, 2016) and reported in d'Amore and Bezzo (2017);
- the spatially-explicit features of the European territory, discretized through a grid  $g = \{1, \dots, 134\}$  of cells as retrieved from d'Amore et al. (2018);
- the techno-economic description through set  $k = \{post_{coal}^{comb}, post_{gas}^{comb}, oxy_{coal}^{fuel}, pre^{comb}\}$  of carbon capture options, that include post-combustion from coal-fired power plants, post-combustion from gas-fired power plants, pre-combustion from gas-fired power plants, and oxy-fuel combustion (d'Amore and Bezzo, 2017);
- the implementation of techno-economic parameters through set  $l = \{pipeline, ship\}$  of transport modes, that include both pipelines (onshore and offshore) and ships; transported flowrates are discretized through a set  $p = \{1, \dots, 7\}$  which ranges from 1 to 30 Mt/year (d'Amore and Bezzo, 2017).
- the location of onshore and offshore basins  $s = \{saline\ aquifer, gas\ field, coal\ field\}$  that are able to efficiently trap the CO<sub>2</sub> for long term geological sequestration, according to data provided by the EU GeoCapacity Project (2009) and mapped in d'Amore et al. (2019);
- the techno-economic features of the CO<sub>2</sub> utilization stage through set  $\psi$  of chemical outputs, which will be described subsequently.

Overall, this European CCUS model is capable of providing:

- the selection, location, scale, and cost of capture nodes;
- the definition, scale, and cost of the transport infrastructure between geographic nodes;
- the location, scale, and cost of geological sequestration nodes;
- the selection, location, scale, and profit of chemical conversion nodes;

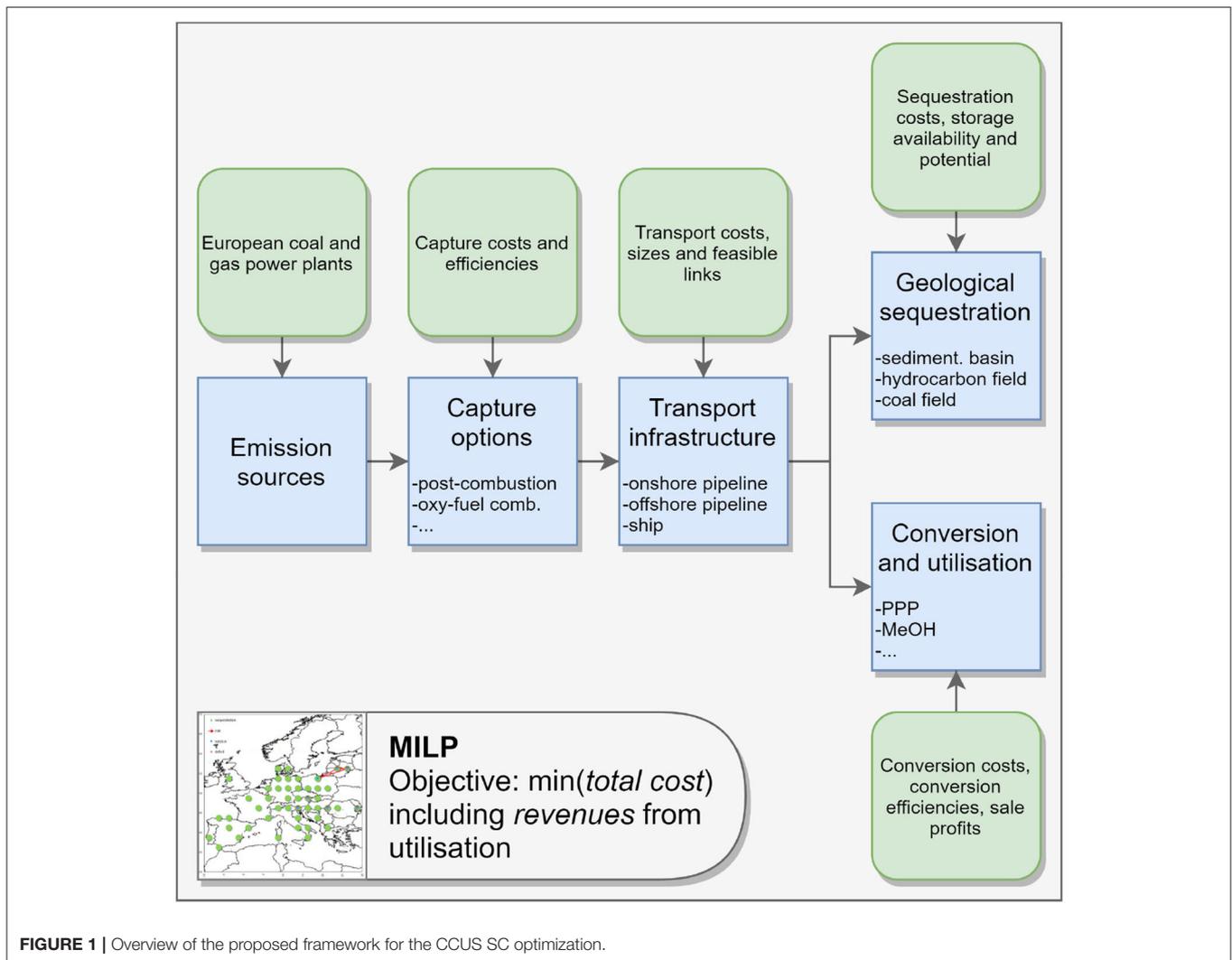


FIGURE 1 | Overview of the proposed framework for the CCUS SC optimization.

- the final CCUS SC configuration according to the chosen European carbon reduction target;
- the differences in SC behavior according to the rates of chemical production;
- the differences in SC behavior according to national regulations on onshore storage.

This study, given the high number of potential reaction mechanisms for CO<sub>2</sub> conversion (Aresta et al., 2013), proposes a screening of the processes according to the following principles:

- (i) *minimum production threshold*: a conversion path is taken into account only if the European demand for the chemical output is a relevant one; the reason for this relies on the large flowrates of CO<sub>2</sub> (i.e.,  $\geq 1$  Mt/year) deriving from stationary sources and consequently on the necessity of exploiting these carbon streams at scale for producing chemicals. Therefore, this model assumes that at least 1 Mt/year of CO<sub>2</sub> should be converted in order to satisfy the market demand;
- (ii) *techno-economic data availability*: the maturity of the technology should be at least such that basic technical (productivity) and economic (production cost) information is available. This means that the current state of research and/or industrial application must be capable of providing complete techno-economic information on the specific conversion process;
- (iii) *environmentally promising*: the conversion process must produce in general less CO<sub>2</sub> than that employed to feed it, thus, the process CO<sub>2</sub> net balance should be negative (i.e., CO<sub>2</sub> emissions are lower than CO<sub>2</sub> consumption); regarding energy requirements, as detailed in the next sections, a first scenario will optimistically assume to exploit only low carbon emission sources (e.g., renewable energy, nuclear energy) to generate the additional electricity required to operate the conversion processes, while a subsequent analysis will take into account the different carbon intensities which are countrywide specific and depend on the local energy mix;

- (iv) *economically promising*: in order to be sustainable from an economic standpoint, the conversion process should be capable of providing a profit from the sale of the chemical output.

As a result, after excluding those products from the CCUS framework, whose processes do not meet the requirements listed above according to information found in the scientific literature (Table 2), two chemical products, i.e., polyether carbonate polyols (PPP) and methanol (MeOH), were selected and included as options for CO<sub>2</sub> utilization in set  $\psi = \{PPP, MeOH\}$ . Regarding the compliance with both the minimum production threshold and the availability of techno-economic data, PPP are bulk chemicals generally employed in the production of polyurethanes and are one of the most commonly produced polymers, with a yearly world production of 9.4 Mt, of which 2.4 Mt is produced just in Europe (Covestro, 2017), whereas MeOH is one of the most versatile and produced chemicals, with a world plant capacity of 125 Mt/year and a European demand of 12 Mt/year (IHS, 2017). When studying the compliance with the environmental requirements, the chemical conversion of CO<sub>2</sub> into PPP (with 20% weight of CO<sub>2</sub>) generates 2.65–2.86 kg CO<sub>2</sub>-eq per kg of product, leading to a GHG emission reduction of about 11% with respect to traditional production technologies (von der Assen and Bardow, 2014). Similarly, the conversion of CO<sub>2</sub> into MeOH allows saving about 1.2 kg of CO<sub>2</sub> per kg of MeOH with respect to its traditional production through steam reforming of natural gas (Roh et al., 2016). According to the literature, the two selected processes for CO<sub>2</sub> chemical conversion are also promising from an economic standpoint. Regarding the conversion of CO<sub>2</sub> into PPP, this process can be specifically designed to generate profits (Fernández-Dacosta et al., 2017), while concerning the production of MeOH, several options have been demonstrated to be economically feasible (e.g., Mondal et al., 2016; Pérez-Fortes et al., 2016; Rivera-Tinoco et al., 2016; Bellotti et al., 2017). It should be noted that the conversion into dimethylcarbonate (DMC), despite looking attractive from both an environmental and an economic point of view (Table 1), does not comply with the minimum production threshold that is imposed here (Covestro, 2017).

### 3. MATHEMATICAL FORMULATION

The objective is to minimize the total cost  $TC$  [€] to install and operate the entire European CCUS network, including the expenditures related to capture facilities  $TCC$  [€], transport infrastructure  $TTC$  [€], and injection of the CO<sub>2</sub> into geological basins  $TSC$  [€], and also considers the *profit* [€] from the utilization stage:

$$\left\{ \begin{array}{l} \text{objective} = \min(TC) \\ TC = TCC + TTC + TSC - \text{profit} \\ \text{s.t.} \\ \text{capture problem model} \\ \text{transport problem model} \\ \text{sequestration problem model} \\ \text{utilization problem model} \end{array} \right. \quad (1)$$

**TABLE 2 |** List of chemicals that can be produced from CO<sub>2</sub> and their effective compliance with the design requirements: (i) minimum production threshold, (ii) techno-economic data availability, (iii) environmentally promising, and (iv) economically promising.

Chemical	References	Compliances			
		(i)	(ii)	(iii)	(iv)
Urea	Heffer and Prud'homme (2016)	V	V	X	V
Polyurethanes	Covestro (2017)	V	V	–	–
Mineral carbonates	Aresta et al. (2013)	V	V	V	X
Syngas	Cairns (2016)	X	V	–	–
MeOH	IHS (2017)	V	V	V	V
Formaldehyde	MC Group (2017)	V	X	–	–
Formic Acid	Aresta et al. (2013)	X	V	V	X
Ethylene	Statista (2013)	X	X	–	–
Ethylene glycol	Aresta et al. (2013)	X	X	–	–
Acetic acid	Aresta et al. (2013)	X	V	–	–
Acrylic acid	Aresta et al. (2013)	X	X	–	–
DMC	Aresta et al. (2013)	X	V	V	V
Salicylic acid	Aresta et al. (2013)	V	X	–	–
Polyoxymethylene	PIE (2016)	X	X	–	–
Polycarbonate	Covestro (2017)	X	X	–	–
Kerosene	CNN (2014)	X	V	V	X
Biodiesel	Lam et al. (2012)	X	V	V	X
Dimethoxyethane	Methanol Institute (2016)	V	X	–	–
Methyl tert-butyl ether	Argus De Witt (2015)	V	X	–	–
PPP	Aresta et al. (2013)	V	V	V	V

Only PPP and MeOH meet all the requirements.

The *capture problem model* entails a set of equations needed to set the optimal captured amounts of CO<sub>2</sub> in regions  $g$  through the most appropriate capture technologies  $k$ , to calculate the value of capture costs  $TCC$ . The *transport problem model* defines the mass balances among regions  $g$  and  $g'$ , to determine the optimal size and routing of the CO<sub>2</sub> flowrates through the different transport means  $l$ , in order to evaluate transport costs  $TTC$ . The *sequestration problem model* describes the optimal positioning of properly sized injection wells in regions  $g$ , to determine costs for storage  $TSC$ . These SC echelons are defined on the basis of techno-economic characteristics of capture options  $k$ , transport modes  $l$ , and sequestration wells, which are all extensively described in d'Amore and Bezzo (2017). In particular, the *capture problem model*, the *transport problem model*, and the *sequestration problem model* have already been discussed in d'Amore and Bezzo (2017) and d'Amore et al. (2018), and their main characteristics are briefly summarized in the **Supplementary Material**. On the other hand, to highlight the key challenge of this contribution, the *utilization problem model* will be entirely described below, on the basis of the conversion processes modeled for producing either PPP (Figure 2A) or MeOH (Figure 2B).

The total *profit* of Equation (1) obtained from the conversion of CO<sub>2</sub> is calculated according to the cash flow  $CF_{\psi,g}$  [€] that can be generated by the production and sale of chemical  $\psi$  in

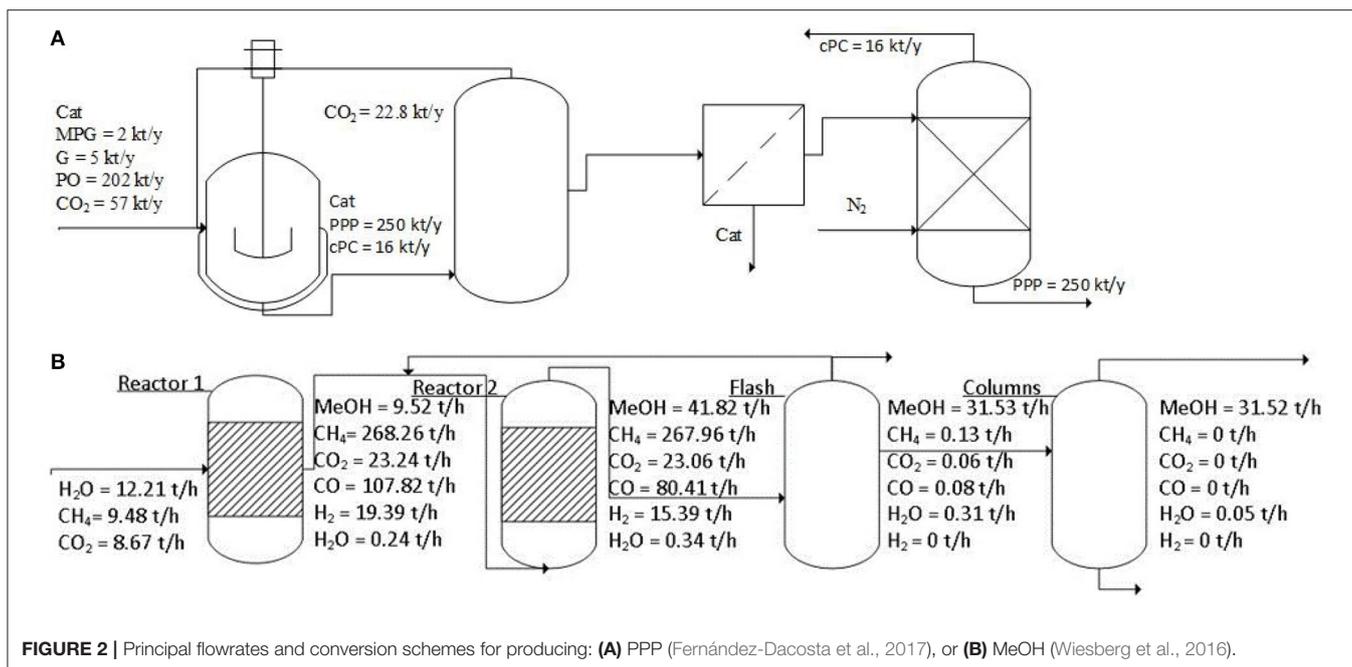


FIGURE 2 | Principal flowrates and conversion schemes for producing: (A) PPP (Fernández-Dacosta et al., 2017), or (B) MeOH (Wiesberg et al., 2016).

region  $g$ :

$$profit = \sum_{\psi,g} CF_{\psi,g} \quad (2)$$

In particular,  $CF_{\psi,g}$  of Equation (2) is defined as:

$$CF_{\psi,g} = (R_{\psi,g} + COM_{\psi,g}) \cdot (1 - tax_g) + d_{\psi,g} \quad \forall \psi, g \quad (3)$$

The revenue  $R_{\psi,g}$  [€] is calculated assuming the sale of both the main product and by-products derived from the production of chemical  $\psi$  in region  $g$ , whereas  $COM_{\psi,g}$  [€] represents the manufacturing cost of chemical  $\psi$  in region  $g$ . Furthermore,  $tax_g$  [%] (Supplementary Table 1 reported in the Supplementary Material) is a country-based parameter that describes the corporate tax rates in each region  $g$ , while  $d_{\psi,g}$  [€] accounts for the depreciation of chemical  $\psi$  in region  $g$ .

As regards the revenue  $R_{\psi,g}$  of Equation (3) of chemical  $\psi$  in region  $g$ , it is given by:

$$R_{\psi,g} = \widehat{R}_{\psi,g} \cdot U_{\psi,g}^{chem} \quad \forall \psi, g \quad (4)$$

where  $U_{\psi,g}^{chem}$  [t] is the amount of chemical  $\psi$  that is produced in region  $g$  as a result of the model solution, whereas  $\widehat{R}_{\psi,g}$  [€/t] is a parameter representing the unitary revenues that can be earned from chemical  $\psi$  in region  $g$ . In particular,  $\widehat{R}_{\psi,g}$  of Equation (4) is calculated according to the unitary price  $P_{\zeta,g}$  [€/t] set on output products  $\zeta$  in region  $g$ , and to the mass flowrates  $\dot{m}_{\zeta,\psi}$  [t/year] of output commodities  $\zeta$  that are generated along with chemical  $\psi$ :

$$\widehat{R}_{\psi,g} = \sum_{\zeta} \frac{P_{\zeta,g} \cdot \dot{m}_{\zeta,\psi}}{U_{\psi}^{ref}} \quad \forall \psi, g \quad (5)$$

The parameter  $U_{\psi}^{ref}$  [set equal to 250 kt/year], representing the reference plant output capacity, the output flowrates  $\dot{m}_{\zeta,\psi}$ , and the unitary prices  $P_{\zeta,\psi}$  set for the production, are retrieved from Souza et al. (2014), Wiesberg et al. (2016), and Fernández-Dacosta et al. (2017), and finally differentiated among the European countries  $c$  according to the different costs of natural gas and electricity (Supplementary Table 1 reported in the Supplementary Material).

The manufacturing cost  $COM_{\psi,g}$  of Equation (3) is calculated according to the formulation proposed by Turton et al. (2015):

$$COM_{\psi,g} = U_{\psi,g}^{chem} \cdot [A^{\psi} \cdot (raw_{\psi,g} + util_{\psi,g})] + B^{\psi} \cdot FCI_{\psi,g} + C^{\psi} \cdot lab_{\psi,g} \cdot \delta_{\psi,g}^{chem} \quad \forall \psi, g \quad (6)$$

Accordingly, the manufacturing cost depends on the amount of chemical  $U_{\psi,g}^{chem}$  of Equation (6), which is multiplied by a scalar  $A^{\psi} = 1.23$ , that conversely weights the sum of  $raw_{\psi,g}$  [€/t] (Supplementary Table 2 reported in the Supplementary Material) and  $util_{\psi,g}$  [€/t] (Supplementary Table 3 reported in the Supplementary Material), these representing the unitary costs of raw materials and utilities for chemical  $\psi$  in region  $g$ , respectively. Furthermore,  $COM_{\psi,g}$  also depends on the fixed capital investment  $FCI_{\psi,g}$  [€] for producing chemical  $\psi$  in region  $g$  (weighted by  $B^{\psi} = 0.28$ ) and on the labor cost  $lab_{\psi,g}$  [€/t] (the latter, reported in Supplementary Table 1, is weighted by  $C^{\psi} = 2.73$ ). The binary variable  $\delta_{\psi,g}^{chem}$  determines whether the productivity  $U_{\psi,g}^{chem}$  of chemical  $\psi$  in region  $g$  falls to a null value, and in that case the contribution of labor costs is also consequently nullified. In fact,  $\delta_{\psi,g}^{chem}$  is a decision variable determining whether there is production of chemical  $\psi$  in region  $g$ , or not, according to the productivity upper bound  $U_{\psi,g}^{max}$  [t

of chemical] (retrieved from IHS, 2017 and Covestro, 2017) of chemical  $\psi$  in region  $g$ :

$$U_{\psi,g}^{chem} \leq \delta_{\psi,g}^{chem} \cdot U_{\psi,g}^{max} \quad \forall \psi, g \quad (7)$$

Regarding the term  $FCI_{\psi,g}$  of Equation (6), it has been evaluated following the non-linear formulation provided by Sinnott and Towler (2009). Then, given the MILP mathematical architecture of this optimization problem, that formulation has been linearized and eventually the following equation has been implemented to calculate  $FCI_{\psi,g}$ , given a non-null amount  $U_{\psi,g}^{chem}$  of chemical  $\psi$  in region  $g$ , and according to the binary decision variable  $\delta_{\psi,g}^{chem}$ :

$$FCI_{\psi,g} = U_{\psi,g}^{chem} \cdot FCI_{\psi}^{slope} + \delta_{\psi,g}^{chem} \cdot FCI_{\psi}^{intercept} \quad \forall \psi, g \quad (8)$$

where  $FCI_{\psi}^{slope}$  [€/t of chemical] and  $FCI_{\psi}^{intercept}$  [€] (Table 3) are respectively the arrays of slope and the intercept coefficients of the linearized facility capital costs for producing each chemical  $\psi$ , and are calculated from the results provided by Aasberg-Petersen et al. (2008).

Having defined  $FCI_{\psi,g}$  through Equation (8), it is then possible to evaluate the depreciation  $d_{\psi,g}$  of Equation (3) of chemical  $\psi$  in region  $g$  as a fixed percentage (set equal to 10% according to d'Amore and Bezzo, 2016) over facility capital cost:

$$d_{\psi,g} = 0.1 \cdot FCI_{\psi,g} \quad \forall \psi, g \quad (9)$$

As seen before in Equations (4), (6),  $U_{\psi,g}^{chem}$  represents the optimal amount of chemical  $\psi$  to be produced in region  $g$  according to the model solution.

It is possible to link the chemical output  $U_{\psi,g}^{chem}$  with the actual CO<sub>2</sub> exploited for utilization, according to the total quantity of CO<sub>2</sub> sent to the conversion process  $U_{\psi,g}$  [t of CO<sub>2</sub>] for producing  $\psi$  in region  $g$ :

$$U_{\psi,g} = U_{\psi,g}^{conv} + U_{\psi,g}^{lost} \quad \forall \psi, g \quad (10)$$

In particular,  $U_{\psi,g}^{conv}$  [t of input CO<sub>2</sub> to the conversion stage] represents the actual quantity of CO<sub>2</sub> that is exploited for conversion and utilization in chemical  $\psi$  in region  $g$ , while  $U_{\psi,g}^{lost}$  [t of emitted CO<sub>2</sub> from the conversion stage] takes into account the direct CO<sub>2</sub> emissions generated by the process when producing chemical  $\psi$  in region  $g$ :

$$U_{\psi,g}^{conv} = \eta_{\psi}^R \cdot U_{\psi,g}^{chem} \quad \forall \psi, g \quad (11)$$

$$U_{\psi,g}^{lost} = (1 - \eta_{\psi}^C) \cdot U_{\psi,g} \quad \forall \psi, g \quad (12)$$

The parameter  $\eta_{\psi}^R$  [t of input CO<sub>2</sub> to the conversion stage/t of chemical  $\psi$ ] (Table 3) of Equation (11) represents the amount of CO<sub>2</sub> that is needed to produce a unitary amount of chemical  $\psi$ . Conversely, the parameter  $\eta_{\psi}^C$  [t of captured CO<sub>2</sub>/t of input CO<sub>2</sub> to the conversion stage] (Table 3) of Equation (12) is introduced to take into account the CO<sub>2</sub> conversion efficiency of the process

**TABLE 3** | Arrays of slopes  $FCI_{\psi}^{slope}$  [€/t of chemical] and intercepts  $FCI_{\psi}^{intercept}$  [€] coefficients for the calculation of the facility capital costs of producing chemical  $\psi$  (Aasberg-Petersen et al., 2008).

	$FCI_{\psi}$				
	Slope [€/t]	Intercept [M€]	$\eta_{\psi}^R$ [t/t]	$\eta_{\psi}^C$ [t/t]	$EEC_{\psi}$ [GJ/t]
PPP	33.96	20.97	0.228	0.6500	0.3754
MeOH	79.79	229.02	1.370	0.9385	29.4000

Carbon quantity  $\eta_{\psi}^R$  [t of input CO<sub>2</sub> to the conversion stage/t of chemical  $\psi$ ] that is reacted and converted to generate chemical  $\psi$ , carbon conversion efficiency  $\eta_{\psi}^C$  [t of captured CO<sub>2</sub>/t of input CO<sub>2</sub> to the conversion stage] in producing chemical  $\psi$ , and electric energy consumption  $EEC_{\psi}$  [GJ/t of input CO<sub>2</sub> to the conversion stage] for producing chemical  $\psi$  (Sakakura and Kohno, 2009; Langanke et al., 2014; Roh et al., 2016; Barbera et al., 2020).

that generates chemical  $\psi$  (Sakakura and Kohno, 2009; Langanke et al., 2014; Roh et al., 2016; Barbera et al., 2020). Given the actually converted CO<sub>2</sub> quantity  $U_{\psi,g}^{conv}$ , it is also possible to evaluate the indirect CO<sub>2</sub> emissions  $U_g^{ind}$  [t of indirect CO<sub>2</sub> from conversion processes]:

$$U_g^{ind} = \sum_{\psi} (CI_g \cdot EEC_{\psi} \cdot U_{\psi,g}^{conv}) \quad \forall g \quad (13)$$

where  $CI_g$  [t of indirect CO<sub>2</sub>/GJ] is the carbon intensity for electricity generation in region  $g$  (Supplementary Table 4 reported in the Supplementary Material) (EEA, 2019; ElectricityMap, 2019; IEA, 2019), whereas  $EEC_{\psi}$  [GJ/t of input CO<sub>2</sub>] (Table 3) is the specific electric energy consumption for producing chemical  $\psi$  (Fernández-Dacosta et al., 2017; Barbera et al., 2020). Note that in case of exploiting only low carbon energy sources (e.g., renewables, nuclear energy) it will be here assumed that  $CI_g = 0$  thus, the contribution of indirect CO<sub>2</sub> emissions generated from conversion processes is completely neglected.

Finally, the total amount of CO<sub>2</sub> converted into chemicals (i.e.,  $U_{\psi,g}^{conv}$ ) is constrained to be larger than that generated by both direct (i.e.,  $U_{\psi,g}^{lost}$ ) and indirect (i.e.,  $U_g^{ind}$ ) emissions produced by the utilization stage:

$$\sum_{\psi,g} U_{\psi,g}^{conv} \geq \sum_{\psi,g} U_{\psi,g}^{lost} + \sum_g U_g^{ind} \quad (14)$$

### 3.1. Scenarios

The time-static CCUS model was optimized using the GAMS CPLEX solver for MILP problems on a 32 GB RAM computer in about 2 h (an optimality gap always lower than 0.5% was reached). Results from the optimal CCS network (hence, without utilization stage) are reported as a matter of comparison (Scenario 0). The CCUS network is here optimized according to the selection of a minimum European reduction target  $\alpha = 50\%$  of overall European CO<sub>2</sub> emissions from large stationary sources, therefore consistent with the recent directives (EC,

**TABLE 4** | Main assumptions and results for Scenario 0, Scenario A, Scenario B, and Scenario C.

Scenario	Model	E. source		Demand	TC [€/t]	TCC [€/t]	TTC [€/t]	TSC [€/t]	profit [€/t]
		ren.	mix						
0	CCS	–	–	–	32.59	30.69	1.64	0.25	–
A <sub>D1</sub>	CCUS	V		1×	31.16	30.77	1.57	0.25	1.44
A <sub>D2</sub>	CCUS	V		2×	29.78	30.80	1.61	0.24	2.87
A <sub>D3</sub>	CCUS	V		3×	28.46	30.86	1.64	0.23	4.27
B	CCUS	V		1×	32.07	30.78	2.32	0.42	1.44
C	CCUS		V	1×	31.90	30.77	1.64	0.25	0.76

All scenarios aim at reaching a European carbon reduction target  $\alpha = 50\%$ . Results are summarized in terms of total cost TC, total capture cost TCC, total transport cost TTC, total sequestration cost TSC, and profit. Intensive values (i.e., [€/t]) refer to the overall sequestered and converted quantity of CO<sub>2</sub>.

2017). Three scenarios have been investigated here (Table 4). In Scenario A<sub>D1</sub> it is assumed that the production of PPP and MeOH cannot be higher than the current European production and that all the electricity needed to perform the conversion and utilization processes comes from zero-carbon energy sources, thus, indirect CO<sub>2</sub> emissions are neglected from the carbon balance and consequently, the constraint imposed through Equation (14) is excluded from the model optimization. Then, Scenario A is also tested on hypothetical higher demands of the two chemicals, i.e., Scenario A<sub>D2</sub> and Scenario A<sub>D3</sub> considering demands that are two and three times, respectively, higher than the current one. A case-study subsequently described, still assuming that no contribution from indirect emissions is accounted for, investigated the fact that some European countries do not allow onshore CO<sub>2</sub> sequestration (Scenario B). Finally, Scenario C analyzes the response of the model to the nationwide characteristics in terms of electricity carbon intensity to determine the optimal CCUS SC while limiting the generation of indirect emissions from conversion and utilization processes therefore, the constraint set by the aim of Equation (14) is included within the model optimization.

## 4. RESULTS

### 4.1. Scenarios A

Scenario A<sub>D1</sub> entails a total cost TC for installing and operating the CCUS SC that is 4.4% lower than that obtained for Scenario 0 (Table 4). This is due to the fact that the introduction of chemical conversion brings in some revenues (the profit in Scenario A<sub>D1</sub> is equal to 1.44 €/t). In particular, the possibility of chemical conversion of CO<sub>2</sub> entails an almost identical capture cost TCC, which slightly increases from 30.69 €/t (Scenario 0) to 30.77 €/t (Scenario A<sub>D1</sub>). On the other hand, Scenario A<sub>D1</sub> exhibits a nearly unchanged transport infrastructure with respect to Scenario 0, despite the necessity of transporting not only the CO<sub>2</sub> that is destined to sequestration, but also the CO<sub>2</sub> fed to the conversion plants (the latter quantity is so small that does not

**TABLE 5** | Main assumptions and results for Scenario 0, Scenario A, Scenario B, and Scenario C.

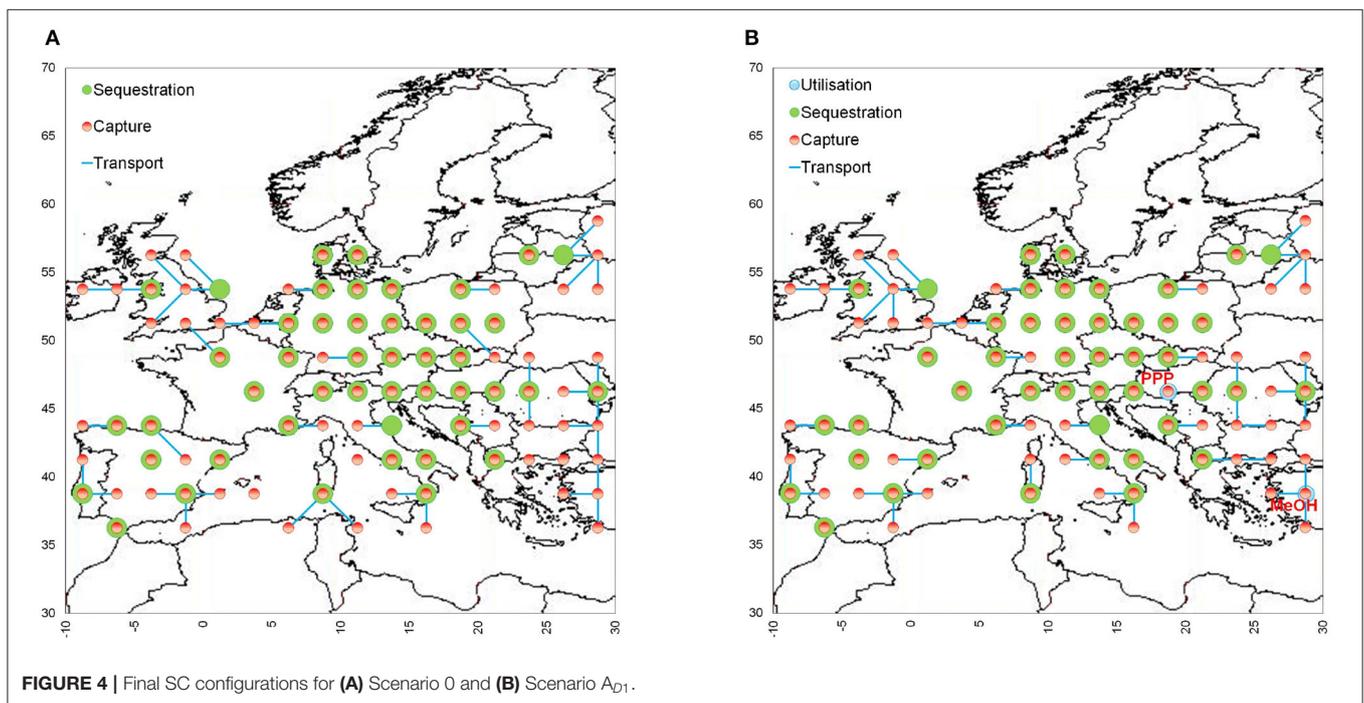
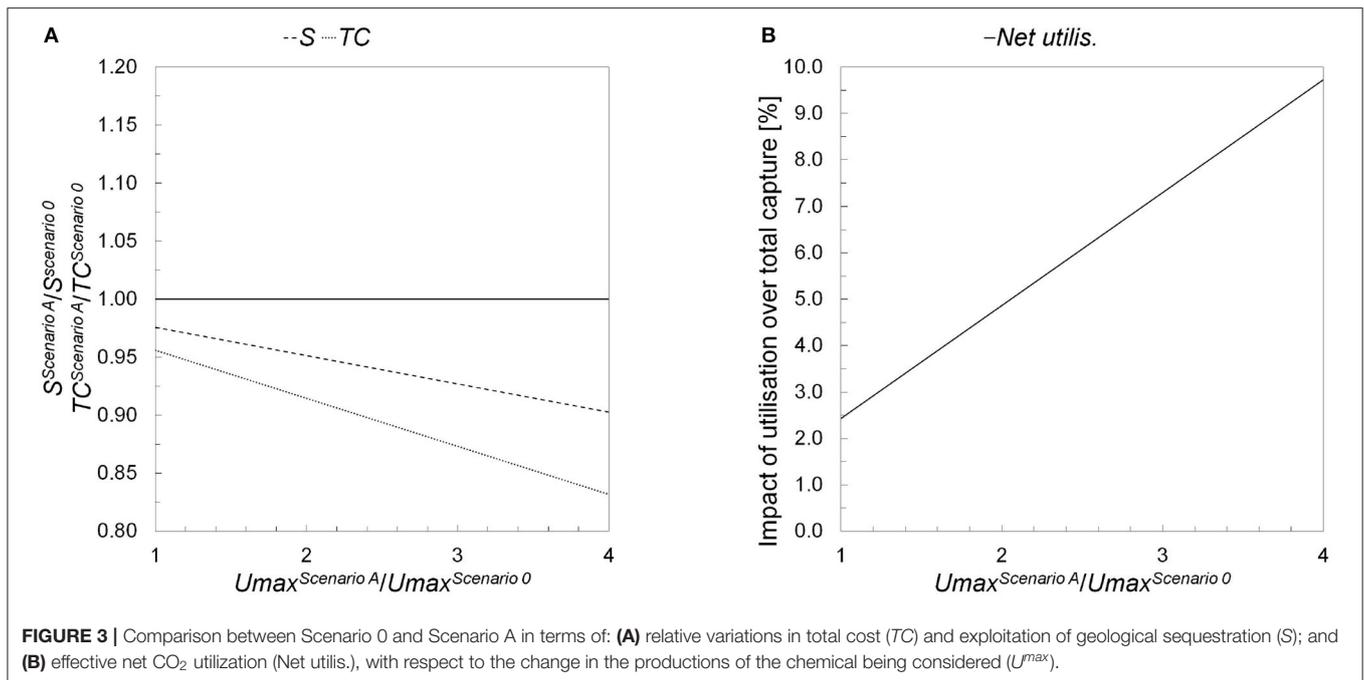
Scenario	Model	E. source		Demand	U <sup>seq</sup> [Mt/year]	U <sup>conv</sup> [Mt/year]	U <sup>lost</sup> [Mt/year]	U <sup>ind</sup> <sub>mix</sub> [Mt/year]
		ren.	mix					
0	CCS	–	–	–	698.57	0.00	0.00	0.00
A <sub>D1</sub>	CCUS	V		1×	681.59	16.99	1.37	64.39
A <sub>D2</sub>	CCUS	V		2×	664.60	33.97	2.74	128.72
A <sub>D3</sub>	CCUS	V		3×	647.61	50.96	4.11	193.06
B	CCUS	V		1×	681.59	16.99	1.37	64.39
C	CCUS		V	1×	681.59	16.99	1.37	15.62

All scenarios aim at reaching a European carbon reduction target  $\alpha = 50\%$ . Results are summarized in terms of yearly sequestered CO<sub>2</sub> U<sup>seq</sup> [Mt/year] yearly converted CO<sub>2</sub> U<sup>conv</sup> [Mt/year], yearly direct CO<sub>2</sub> emissions due to conversion processes U<sup>lost</sup> [Mt/year], and yearly indirect CO<sub>2</sub> emissions due to conversion processes (if local energy mixes were/are considered) U<sup>ind</sup><sub>mix</sub> [Mt/year].

affect the overall structure of the transport network). This result is not surprising if we consider that the same total quantity of CO<sub>2</sub> is imposed to be captured from stationary sources in all scenarios, and therefore the same total flowrate must be shipped between the nodes (independently of the choice of either sequestration or utilization). As a result, the total transport cost TTC just slightly varies from 1.64 €/t (Scenario 0) to 1.57 €/t (Scenario A<sub>D1</sub>). The exploitation of geological storage slightly diminishes with respect to Scenario 0 (i.e., –2.43%) (Table 5). Total sequestration costs TSC are unchanged between Scenario 0 and Scenario A<sub>D1</sub> (0.25 €/t). The net impact of utilization amounts to 2.43% of the overall captured CO<sub>2</sub> therefore, the result is comparable with the 1% upper bound for chemical conversion estimated by Mac Dowell et al. (2017).

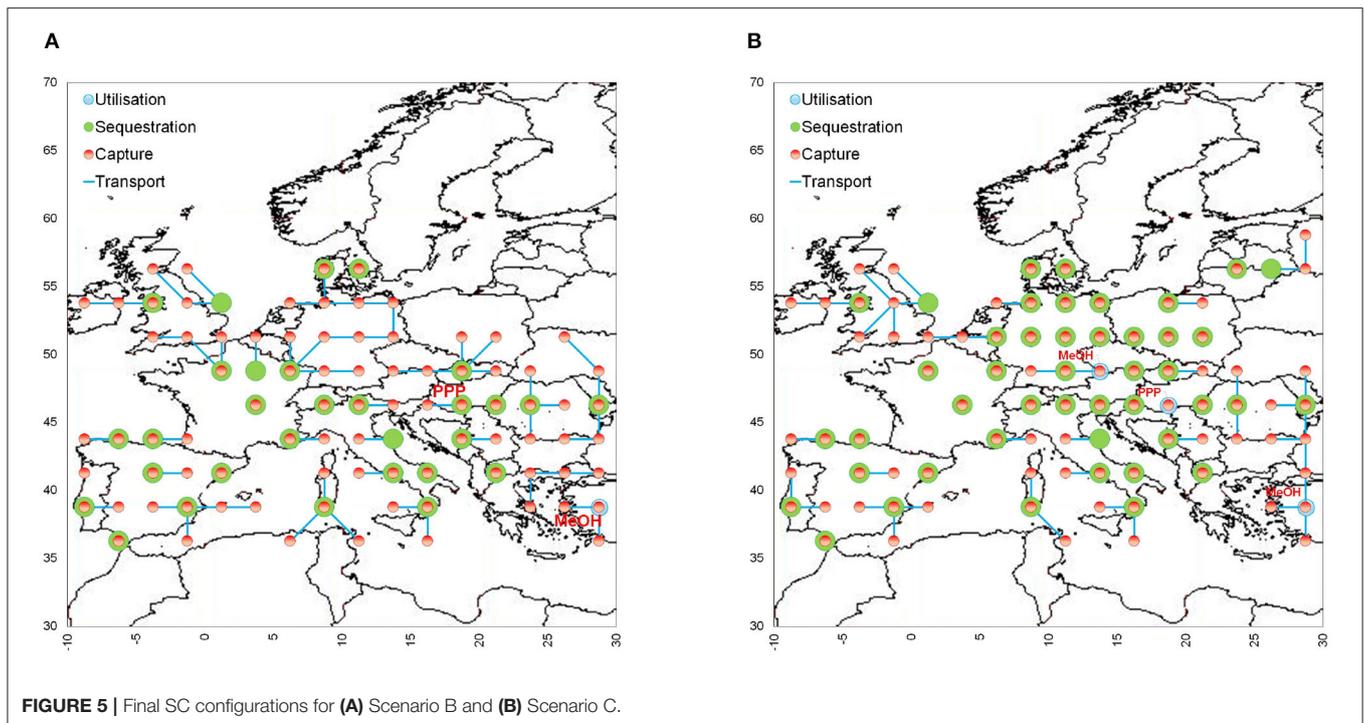
Scenario A<sub>D2</sub> and Scenario A<sub>D3</sub> focus on investigating how the cost of a CO<sub>2</sub> SC would vary if the production of chemicals was increased progressively from the current European values (i.e., with respect to Scenario A<sub>D1</sub>) to three times that (Tables 4, 5). Accordingly, tripling the production of both chemicals corresponds to an increase of the European production quota from 25.5%<sup>PPP</sup> and 9.6%<sup>MeOH</sup> (Scenario A<sub>D1</sub>) to 76.6%<sup>PPP</sup> and 28.8%<sup>MeOH</sup> (Scenario A<sub>D3</sub>) of actual world capacity. Under these assumptions, the results from the optimal CCUS configuration show that overproduction of the two chemicals mainly affects the total cost of the SC, which could be reduced by about 12.67% in case the production of both chemicals was tripled with respect to current values. On the other hand, the contribution of CO<sub>2</sub> utilization over capture would go from 2.43% (Scenario A<sub>D1</sub>) to a maximum of about 7.29% (Scenario A<sub>D3</sub>) (Figure 3A). This means that, in order to completely avoid the necessity of CO<sub>2</sub> sequestration, a massive increase to over 38 times the current European production of PPP and MeOH would be required. In terms of GHGs savings, Scenario A<sub>D3</sub> would allow a net CO<sub>2</sub> yearly decrease due to utilization equal to 50.96 Mt/year, against just 16.99 Mt/year for Scenario A<sub>D1</sub> (Figure 3B).

The final SC configuration is reported in Figure 4 for both Scenario 0 (Figure 4A) and Scenario A<sub>D1</sub> (Figure 4B). Note that



for the cases of Scenario  $A_{D2-D3}$  the SC design is unchanged with respect to Scenario  $A_{D1}$ , since varying the demands of the two chemicals only determines the installation of larger conversion facilities, while their location and infrastructure is not affected. **Figure 4** highlights that the resulting networks are almost identical between Scenario 0 and Scenario  $A_{D1}$ . Capture nodes do not change and, consequently, the main driver in establishing the transportation arcs is the location

of the sequestration sites. Regarding the utilization stage, the conversion facilities are located in regions allowing for a reduction of production costs, i.e., Hungary (PPP) and Turkey (MeOH). In fact, it was verified that the key parameters affecting the selection of the plant sites are corporate tax rate, cost of materials, and energy price. Regarding corporate tax rates, there is a large variability across Europe (**Supplementary Table 1** reported in the **Supplementary Material**), from a minimum



**FIGURE 5** | Final SC configurations for (A) Scenario B and (B) Scenario C.

of 9% (Hungary) up to a maximum of 34% (Belgium). The corporate tax rate of Macedonia is just slightly higher than that of Hungary, while the one of Turkey is close to the European mean (i.e., 20%). As a consequence, the construction of plants in Hungary is mainly justified by their competitiveness in corporate tax rates. On the other hand, Turkey is characterized by low costs of raw materials (**Supplementary Table 2** reported in the **Supplementary Material**) and utilities (**Supplementary Table 3** reported in the **Supplementary Material**). In particular, Turkey has the cheapest electricity price among the analyzed countries (0.0187 €/kWh) (**Supplementary Table 1** reported in the **Supplementary Material**). Accordingly, the presence of a plant for producing MeOH in Turkey is quite justifiable despite the high energy intensity required by its production process. Summarizing, the location of plants for CO<sub>2</sub> conversion into PPP is mainly driven by low taxation, since this process is less energy intensive. Conversely, regarding the production of MeOH, its optimal positioning is mainly determined by the cost of raw materials and utilities (and, in particular, of electricity). Labor costs do not seem to have a relevant impact for choosing the locations of CO<sub>2</sub> conversion facilities.

## 4.2. Scenario B

Scenario B considers the fact that some countries restrict (Czech Republic, Germany, Poland, Sweden, the Netherlands, and the United Kingdom) or forbid (Austria, Croatia, Estonia, Ireland, Latvia, Finland, and Belgium) onshore sequestration (EC, 2017). Even though the United Kingdom, Poland, and the Netherlands are in the process of authorizing it (EC, 2017), Scenario B prudently optimizes the CCUS SC while excluding all the aforementioned states from those in which onshore

storage is allowed. Results show that the total cost *TC* does not change significantly (about 3% more expensive with respect to Scenario A<sub>D1</sub>), while capture costs *TCC* and *profit* are also unchanged between the two analyzed case studies (**Table 4**). On the other hand, analogously to that observed in d'Amore and Bezzo (2017) for CCS SCs, the optimal CCUS network entails a more complex and expensive transport infrastructure (+48% in terms of *TTC*) and sequestration stage (+68% in terms of *TSC*). These additional expenditures are a consequence of the necessity of routing CO<sub>2</sub> flowrates toward those sequestration basins that are still available once countrywide legal frameworks are taken into account (**Figure 4A**). Regarding the CO<sub>2</sub> exploited for conversion and utilization purposes, the restrictive legal framework for onshore storage produces the same identical results obtained in Scenario A<sub>D1</sub>.

## 4.3. Scenario C

The previously discussed scenarios A-B investigated the design of optimal European CCUS SCs while neglecting the indirect CO<sub>2</sub> emissions that may be generated by the energy requirements of conversion processes. As shown in **Table 5**, if these network considered the contribution of the local energy mixes toward indirect emissions from chemicals production, the overall amount of CO<sub>2</sub> generated (directly and indirectly from its conversion) would be higher than that captured. To overcome this simplification, which may lead to unrealistic results, Scenario C optimizes the European CCUS network while taking into account the country-specific electricity carbon intensities. As a result, most of the production of MeOH is now located in Austria, which is a country characterized by a particularly attractive compromise between a low electricity carbon intensity (i.e.,

0.024 t of CO<sub>2</sub>/GJ) and production cost parameters (Figure 5B). As in Scenario A<sub>D1</sub>, a residual production of MeOH is still located in Turkey and a PPP plant is installed in Hungary. The drawback of keeping net CO<sub>2</sub> emissions negative lays on the slight increase in total costs *TC* (+2.4% with respect to Scenario A<sub>D1</sub>), which is due to a drop in total *profit* earned from the sale of chemical outputs (−47.2% with respect to Scenario A<sub>D1</sub>) (Table 4). Overall, Scenario C demonstrates that indirect CO<sub>2</sub> emissions generated from CO<sub>2</sub> conversion processes (i.e.,  $U^{ind}$ ) might play a key role in determining the economics and design of a European CCUS network, but that in general, a satisfactory solution entailing negative CO<sub>2</sub> emissions can be obtained while still generating some profit from both PPP and MeOH. Moreover, the contribution of direct additional CO<sub>2</sub> emissions from utilization (i.e.,  $U^{lost}$ ) was always negligible in all analyzed scenarios.

## 5. DISCUSSION

Results of the optimization show that for the case study being considered, CO<sub>2</sub> utilization may have a non-negligible economic impact (overall costs decrease by 4.4%); however, as suggested by other studies (e.g., Mac Dowell et al., 2017), its environmental impact is a minor one (in our case study, the contribution amounts to 2.4% reduction in GHGs emissions). Thus, the major benefit of CO<sub>2</sub> utilization seems to be that of a slight reduction in taxpayer costs in establishing a CCS infrastructure.

Having stated that, we need to highlight the limitations, too, of this study. First, the focus was on the very few chemical technologies that are currently demonstrated to be sufficiently mature to provide a reduction in CO<sub>2</sub> emissions, and to guarantee some profitability. Although material balances (Mac Dowell et al., 2017) and thermodynamics (Stevenson, 2019) still limit the potential of the chemical industry in terms of CO<sub>2</sub> utilization, alternative pathways may nonetheless disclose wider and more positive scenarios. For instance the application of CCU technologies in the cement industry could foster the routing toward an “ideally carbon-free” market in which construction materials are generated from the same CO<sub>2</sub> captured within the plant itself or from large stationary sources (US National Academy of Sciences, 2019). Furthermore, this study does not consider the possibility that the unsatisfactory environmental performance of a technology could be balanced by negative emissions in a different location, thanks to some sort of carbon trading mechanisms or cooperative actions. Similarly we did not consider the possibility of favorable local situations (e.g., a conversion facility fed by renewable power plant producing electricity at a cheap price), which could change the economic and/or environmental sustainability of some technologies in some specific cases. The energy sector, too, may provide a huge market for CO<sub>2</sub>-derived fuels. As a matter of fact, methanol is currently envisioned for a wide range of applications beyond its current use, e.g., as fuel for transport, in energy sectors, or for the synthesis of hydrocarbons, including several major large-volume chemicals (Pérez-Forbes et al., 2016). Hence, imposing the current production volumes

as an upper bound for the calculation of utilization potential may neglect a wide range of additional options. Furthermore, focusing on large stationary sources may neglect the fact that more effective conversion routes could be established at an industrial level, e.g., by integrating conversion technologies within a petrochemical plant. Governmental subsidies, too, may help support some technologies and accelerate the transition toward a CO<sub>2</sub> derived chemical industry. However, the definition of the most suitable mechanisms and their effect on the deployment of alternative technologies is beyond the scope of this work. We need to recognize, though, that currently, many potential routes are just possibilities and that their practical implementation is far from being demonstrated at a large scale (US National Academy of Sciences, 2019): the degree of uncertainty in terms of costs, productivity, GHGs emissions is so high that any modeling and optimization framework may simply result in a speculative exercise with questionable practical benefits. This is why we decided to exclude such routes in the current analysis.

On the other hand, even our “conservative” approach could be alleged by someone to be over-optimistic. In fact, it is assumed that traditional routes for the chemicals being considered would move to alternative technologies based on CO<sub>2</sub> conversion so that all European production would rely on CO<sub>2</sub> as a feedstock. In the current situation, such a scenario does not appear to be very plausible unless significant incentives are introduced or whole world production follows a similar path.

To sum up, even if there are limitations, we believe that the proposed analysis may represent a sound preliminary assessment of current potential of CCUS in Europe, when CO<sub>2</sub> emissions from large stationary sources are taken into account.

## 6. CONCLUSIONS

This article assessed the potential impact of a European carbon capture, transport, utilization, and storage supply chain. Results suggested that CO<sub>2</sub> utilization can contribute only marginally to achieve the European climate target set for 2030 in terms of emissions reduction. The positive effect is that it can generate some profits and consequently help to decrease costs related to the overall carbon capture and sequestration infrastructure. Moreover, this analysis demonstrated the key role played by national energy mixes (thus, energy carbon intensities) in determining the optimal positioning of conversion plants as a consequence of accounting for both direct and indirect CO<sub>2</sub> emissions from the conversion stage; furthermore, the study was able to show the response in terms of a network design to countrywide legal frameworks on onshore geological storage.

This work sets the basis for future research on the strategic optimization of carbon capture, transport, utilization, and sequestration supply chains at a wide continent-level scale. The proposed methodology is general, since it could be applied to different geographic contexts, and could be

improved by adding more CO<sub>2</sub> conversion and utilization pathways, in order to achieve a more comprehensive modeling framework.

## DATA AVAILABILITY STATEMENT

All datasets generated for this study are either included in the article/**Supplementary Material**, or available upon request to the corresponding author.

## AUTHOR CONTRIBUTIONS

FB conceived and led this study. Fd'A developed the model formulation and implementation, carried out the analyses, and wrote the paper. Fd'A and FB contributed to the text and edited the paper. All authors contributed to the article and approved the submitted version.

## REFERENCES

- Aasberg-Petersen, K., Nielsen, C. S., Dybkjær, I., and Perregaard, J. (2008). *Large Scale Methanol Production From Natural Gas*. Haldor Topsoe, 22. Available online at: [http://www.topsoe.com/sites/default/files/topsoe\\_large\\_scale\\_methanol\\_prod\\_paper.ashx.pdf](http://www.topsoe.com/sites/default/files/topsoe_large_scale_methanol_prod_paper.ashx.pdf) (accessed March 29, 2018).
- Agrali, S., Üçtuğ, F. G., and Türkmen, B. A. (2018). An optimization model for carbon capture and storage/utilization vs. carbon trading: a case study of fossil-fired power plants in Turkey. *J. Environ. Manage.* 215, 305–315. doi: 10.1016/j.jenvman.2018.03.054
- Alper, E., and Yuksel Orhan, O. (2017). CO<sub>2</sub> utilization: developments in conversion processes. *Petroleum* 3, 109–126. doi: 10.1016/j.petlm.2016.11.003
- Aresta, M., Dibenedetto, A., and Angelini, A. (2013). The changing paradigm in CO<sub>2</sub> utilization. *J. CO<sub>2</sub> Util.* 3–4, 65–73. doi: 10.1016/j.jcou.2013.08.001
- Argus De Witt, A. (2015). *Argus DeWitt 2015 Fuels and Oxygenates Annual*. Available online at: <https://www.argusmedia.com/~media/files/pdfs/ptchems/mtbe-2015-annual-flyer.pdf?la=en> (accessed March 29, 2018).
- Armstrong, K., and Styring, P. (2015). Assessing the potential of utilization and storage strategies for post-combustion CO<sub>2</sub> emissions reduction. *Front. Energy Res.* 3, 1–9. doi: 10.3389/fenrg.2015.00008
- Barbera, E., Mantoan, F., Bertuccio, A., and Bezzo, F. (2020). Hydrogenation to convert CO<sub>2</sub> to C1 chemicals: technical comparison of different alternatives by process simulation. *Can. J. Chem. Eng.* 98, 1893–1906. doi: 10.1002/cjce.23755
- Bellotti, D., Rivarolo, M., Magistri, L., and Massardo, A. F. (2017). Feasibility study of methanol production plant from hydrogen and captured carbon dioxide. *J. CO<sub>2</sub> Util.* 21, 132–138. doi: 10.1016/j.jcou.2017.07.001
- Bui, M., Adjiman, C. S., Bardow, A., Anthony, E. J., Boston, A., Brown, S., et al. (2018). Carbon capture and storage (CCS): the way forward. *Energy Environ. Sci.* 11, 1062–1176. doi: 10.1039/c7ee02342a
- Cairns, H. (2016). *Global Trends in Syngas*, Technical report. Stratas Advisors. Available online at: <https://stratasadvisors.com/Insights/072216-Global-Syngas-Trends> (accessed September 15, 2020).
- CNN (2014). *Desert Plants and Green Diesel: Meet the Jet Fuels of the Future*. Available online at: <http://edition.cnn.com/travel/article/boeing-biofuel/index.html> (accessed September 15, 2020)
- Covestro (2017). *Investor Presentation Technical Report*. Available online at: <http://investor.covestro.com/en/presentations/presentations/> (accessed September 15, 2020)
- d'Amore, F., and Bezzo, F. (2016). Strategic optimisation of biomass-based energy supply chains for sustainable mobility. *Comput. Chem. Eng.* 87, 68–81. doi: 10.1016/j.compchemeng.2016.01.003
- d'Amore, F., and Bezzo, F. (2017). Economic optimisation of European supply chains for CO<sub>2</sub> capture, transport and sequestration. *Int. J. Greenh. Gas Control* 65, 99–116. doi: 10.1016/j.ijggc.2017.08.015
- d'Amore, F., and Bezzo, F. (2020). Optimal design of European cooperative supply chains for carbon capture, transport and sequestration with costs share policies. *AIChE J.* 66:e16872. doi: 10.1002/AIC.16872
- d'Amore, F., Lovisotto, L., and Bezzo, F. (2020). Introducing social acceptance into the design of CCS supply chains: a case study at a European level. *J. Clean. Prod.* 249:119337. doi: 10.1016/j.jclepro.2019.119337
- d'Amore, F., Mocellin, P., Vianello, C., Maschio, G., and Bezzo, F. (2018). Economic optimisation of European supply chains for CO<sub>2</sub> capture, transport and sequestration, including societal risk analysis and risk mitigation measures. *Appl. Energy* 223, 401–415. doi: 10.1016/j.apenergy.2018.04.043
- d'Amore, F., Sunny, N., Iruretagoyena, D., Bezzo, F., and Shah, N. (2019). European supply chains for carbon capture, transport and sequestration, with uncertainties in geological storage capacity: insights from economic optimisation. *Comput. Chem. Eng.* 129:106521. doi: 10.1016/j.compchemeng.2019.106521
- EC (2017). *Report From the Commission to the European Parliament and the Council on Implementation of Directive 2009/31/EC on the Geological Storage of Carbon Dioxide*. Available online at: [https://ec.europa.eu/commission/sites/beta-political/files/report-carbon-capture-storage\\_en.pdf](https://ec.europa.eu/commission/sites/beta-political/files/report-carbon-capture-storage_en.pdf) (accessed September 15, 2020)
- EEA (2019). *CO<sub>2</sub> Emission Intensity*. Available online at: <https://www.eea.europa.eu/data-and-maps> (accessed September 15, 2020)
- Elahi, N., Shah, N., Korre, A., and Durucan, S. (2014). Multi-period least cost optimisation model of an integrated carbon dioxide capture transportation and storage infrastructure in the UK. *Energy Procedia* 63, 2655–2662. doi: 10.1016/j.egypro.2014.11.288
- Elahi, N., Shah, N., Korre, A., and Durucan, S. (2017). Multi-stage stochastic optimisation of a CO<sub>2</sub> transport and geological storage in the UK. *Energy Procedia* 114, 6514–6525. doi: 10.1016/j.egypro.2017.03.1787
- ElectricityMap (2019). *Climate Impact by Area: Ranked by Carbon Intensity of Electricity Consumed*. Available online at: <https://www.electricitymap.org/> (accessed September 15, 2020)
- EU GeoCapacity Project (2009). *Assessing European Capacity for Geological Storage of Carbon Dioxide*. Available online at: [www.geology.cz/geocapacity/publications/](http://www.geology.cz/geocapacity/publications/) (accessed September 15, 2020)
- Eurostat (2017a). *Energy Price Statistics*. Available online at: [http://ec.europa.eu/eurostat/statistics-explained/index.php/Energy\\_price\\_statistics](http://ec.europa.eu/eurostat/statistics-explained/index.php/Energy_price_statistics) (accessed September 15, 2020)

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## SUPPLEMENTARY MATERIAL

The Supplementary Material for this article can be found online at: <https://www.frontiersin.org/articles/10.3389/fenrg.2020.00190/full#supplementary-material>

- Eurostat (2017b). *Labour Costs Database*. Available online at: <http://ec.europa.eu/eurostat/web/labour-market/labour-costs/database> (accessed September 15, 2020)
- Eurostat (2017c). *Natural Gas Price Statistics*. Available online at: [http://ec.europa.eu/eurostat/statistics-explained/index.php/Natural\\_gas\\_price\\_statistics](http://ec.europa.eu/eurostat/statistics-explained/index.php/Natural_gas_price_statistics) (accessed September 15, 2020)
- Fernández-Dacosta, C., Van Der Spek, M., Hung, C. R., Oregioni, G. D., Skagestad, R., Parihar, P., et al. (2017). Prospective techno-economic and environmental assessment of carbon capture at a refinery and CO<sub>2</sub> utilisation in polyol synthesis. *J. CO<sub>2</sub> Util.* 21, 405–422. doi: 10.1016/j.jcou.2017.08.005
- Geske, J., Berghout, N., and van den Broek, M. (2015). Cost-effective balance between CO<sub>2</sub> vessel and pipeline transport: part II—design of multimodal CO<sub>2</sub> transport: the case of the West Mediterranean region. *Int. J. Greenh. Gas Control* 33, 122–134. doi: 10.1016/j.ijggc.2014.12.005
- Han, J. H., and Lee, I. B. (2012). Multiperiod stochastic optimization model for carbon capture and storage infrastructure under uncertainty in CO<sub>2</sub> emissions, product prices, and operating costs. *Ind. Eng. Chem. Res.* 51, 11445–11457. doi: 10.1021/ie3004754
- Han, J. H., and Lee, I. B. (2013). A comprehensive infrastructure assessment model for carbon capture and storage responding to climate change under uncertainty. *Ind. Eng. Chem. Res.* 52, 3805–3815. doi: 10.1021/ie301451e
- Hasan, M. M. F., First, E. L., Boukouvala, F., and Floudas, C. A. (2015). A multi-scale framework for CO<sub>2</sub> capture, utilization, and sequestration: CCUS and CCU. *Comput. Chem. Eng.* 81, 2–21. doi: 10.1016/j.compchemeng.2015.04.034
- Heffer, P., and Prud'homme, M. (2016). "Fertilizer outlook 2016–2020," in *84th IFA Annual Conference, Moscow, 30 May–1 June 2016* (Moscow: International Fertilizer Industry Association (IFA)).
- IEA (2019). *Data and Statistics: Explore Energy Data by Category, Indicator, Country or Region*. Available online at: <https://www.iea.org/data-and-statistics> (accessed September 15, 2020)
- IHS (2017). *Global Methanol Demand Growth Driven by Methanol to Olefins as Chinese Thirst for Chemical Supply Grows*. IHS Markit Says. Available online at: <http://news.ihsmarkit.com/press-release/country-industry-forecasting-media/global-methanol-demand-growth-driven-methanol-olefi> (accessed September 15, 2020)
- IPCC (2005). *IPCC Special Report on Carbon Dioxide Capture and Storage. Prepared by Working Group III of the Intergovernmental Panel on Climate Change*. Cambridge University Press, 442. Available online at: [https://www.ipcc.ch/pdf/special-reports/srccs/srccs\\_wholereport.pdf](https://www.ipcc.ch/pdf/special-reports/srccs/srccs_wholereport.pdf) (accessed September 15, 2020)
- IPCC (2018). *Global Warming of 1.5°C. An IPCC Special Report on the Impacts of Global Warming of 1.5°C Above Pre-industrial Levels and Related Global Greenhouse Gas Emission Pathways, in the Context of Strengthening the Global Response to the Threat of Climate Change*. Available online at: [http://report.ipcc.ch/sr15/pdf/sr15\\_spm\\_final.pdf](http://report.ipcc.ch/sr15/pdf/sr15_spm_final.pdf) (accessed September 15, 2020)
- JRC (2016). *Emission Database for Global Atmospheric Research (EDGAR)*. Available online at: [edgar.jrc.ec.europa.eu/index.php](http://edgar.jrc.ec.europa.eu/index.php) (accessed September 15, 2020)
- Kalyanarengan Ravi, N., Van Sint Annaland, M., Fransoo, J. C., Grievink, J., and Zondervan, E. (2016). Development and implementation of supply chain optimization framework for CO<sub>2</sub> capture and storage in the Netherlands. *Comput. Chem. Eng.* 102, 40–51. doi: 10.1016/j.compchemeng.2016.08.011
- Kim, M., Kim, K., Kim, T. H., and Kim, J. (2019). Economic and environmental benefit analysis of a renewable energy supply system integrated with carbon capture and utilization framework. *Chem. Eng. Res. Des.* 147, 200–213. doi: 10.1016/j.cherd.2019.05.008
- Klokk, Ø., Schreiner, P. F., Pagès-Bernaus, A., and Tomsgard, A. (2010). Optimizing a CO<sub>2</sub> value chain for the Norwegian continental shelf. *Energy Policy* 38, 6604–6614. doi: 10.1016/j.enpol.2010.06.031
- Lam, M. K., Lee, K. T., and Mohamed, A. R. (2012). Current status and challenges on microalgae-based carbon capture. *Int. J. Greenh. Gas Control* 10, 456–469. doi: 10.1016/j.ijggc.2012.07.010
- Langanke, J., Wolf, A., Hofmann, J., Böhm, K., Subhani, M. A., Müller, T. E., et al. (2014). Carbon dioxide (CO<sub>2</sub>) as sustainable feedstock for polyurethane production. *Green Chem.* 16, 1865–1870. doi: 10.1039/C3GC41788C
- Lee, S. Y., Lee, I. B., and Han, J. (2019). Design under uncertainty of carbon capture, utilization and storage infrastructure considering profit, environmental impact, and risk preference. *Appl. Energy* 238, 34–44. doi: 10.1016/j.apenergy.2019.01.058
- Lee, S. Y., Lee, J. U., Lee, I. B., and Han, J. (2017). Design under uncertainty of carbon capture and storage infrastructure considering cost, environmental impact, and preference on risk. *Appl. Energy* 189, 725–738. doi: 10.1016/j.apenergy.2016.12.066
- Lehtonen, J., Järnefelt, V., Alakurtti, S., Arasto, A., Hannula, I., Harlin, A., et al. (2019). *The Carbon Reuse Economy: Transforming CO<sub>2</sub> From a Pollutant Into a Resource*. Espoo: VTT Technical Research Centre of Finland.
- Leonzio, G., Foscolo, P. U., and Zondervan, E. (2019). An outlook towards 2030: optimization and design of a CCUS supply chain in Germany. *Comput. Chem. Eng.* 125, 499–513. doi: 10.1016/j.compchemeng.2019.04.001
- Li, H., Jiang, H. D., Yang, B., and Liao, H. (2019). An analysis of research hotspots and modeling techniques on carbon capture and storage. *Sci. Total Environ.* 687, 687–701. doi: 10.1016/j.scitotenv.2019.06.013
- Mac Dowell, N., Fennell, P. S., Shah, N., and Maitland, G. C. (2017). The role of CO<sub>2</sub> capture and utilization in mitigating climate change. *Nat. Clim. Change* 7, 243–249. doi: 10.1038/nclimate3231
- MC Group (2017). *World Formaldehyde Production to Exceed 52 Mln Tonnes in 2017*. Available online at: <https://mcgroup.co.uk/news/20140627/formaldehyde-production-exceed-52-mln-tonnes.html> (accessed September 15, 2020)
- Methanol Institute (2016). *DME: An Emerging Global Fuel*, Technical report. Available online at: <http://www.methanol.org/wp-content/uploads/2016/06/DME-An-Emerging-Global-Guel-FS.pdf>
- Middleton, R. S., Keating, G. N., Viswanathan, H. S., Stauffer, P. H., and Pawar, R. J. (2012). Effects of geologic reservoir uncertainty on CO<sub>2</sub> transport and storage infrastructure. *Int. J. Greenh. Gas Control* 8, 132–142. doi: 10.1016/j.ijggc.2012.02.005
- Middleton, R. S., and Yaw, S. (2018). The cost of getting CCS wrong: uncertainty, infrastructure design, and stranded CO<sub>2</sub>. *Int. J. Greenh. Gas Control* 70, 1–11. doi: 10.1016/j.ijggc.2017.12.011
- Mondal, K., Sasmal, S., Badgandi, S., Chowdhury, D. R., and Nair, V. (2016). Dry reforming of methane to syngas: a potential alternative process for value added chemicals—a techno-economic perspective. *Environ. Sci. Pollut. Res.* 23, 22267–22273. doi: 10.1007/s11356-016-6310-4
- Nie, Z., Korre, A., Elahi, N., and Durucan, S. (2017). Real options analysis of CO<sub>2</sub> transport and storage in the UK continental shelf under geological and market uncertainties and the viability of subsidies for market development. *Energy Procedia* 114, 6612–6622. doi: 10.1016/j.egypro.2017.03.1815
- Pérez-Fortes, M., Schöneberger, J. C., Boulamanti, A., and Tzimas, E. (2016). Methanol synthesis using captured CO<sub>2</sub> as raw material: techno-economic and environmental assessment. *Appl. Energy* 161, 718–732. doi: 10.1016/j.apenergy.2015.07.067
- PIE (2016). *POM Technical Report*. Available online at: <https://pieweb.plasteurope.com/Default.aspx?pageid=302&node=100212> (accessed September 15, 2020)
- Rivera-Tinoco, R., Farran, M., Bouallou, C., Auprêtre, F., Valentin, S., Millet, P., et al. (2016). Investigation of power-to-methanol processes coupling electrolytic hydrogen production and catalytic CO<sub>2</sub> reduction. *Int. J. Hydrogen Energy* 41, 4546–4559. doi: 10.1016/j.ijhydene.2016.01.059
- Roh, K., Frauzem, R., Nguyen, T. B. H., Gani, R., and Lee, J. H. (2016). A methodology for the sustainable design and implementation strategy of CO<sub>2</sub> utilization processes. *Comput. Chem. Eng.* 91, 407–421. doi: 10.1016/j.compchemeng.2016.01.019
- Sakakura, T., and Kohno, K. (2009). The synthesis of organic carbonates from carbon dioxide. *Chem. Commun.* 11, 1312–1330. doi: 10.1039/b819997c
- Sinnot, R., and Towler, G. (2009). *Chemical Engineering Design. 5th Edn* (Oxford: Butterworth-Heinemann).
- Smit, B., Park, A. H. A., and Gadikota, G. (2014). The grand challenges in carbon capture, utilization, and storage. *Front. Energy Res.* 2, 2013–2015. doi: 10.3389/fenrg.2014.00055
- Souza, L. F. S., Ferreira, P. R. R., Medeiros, J. L. De, Alves, R. M. B., and Arau, Q. F. (2014). Production of DMC from CO<sub>2</sub> via indirect route: technical–environmental–assessment and analysis. *ACS Sustain. Chem. Eng.* 2, 62–69. doi: 10.1021/sc400279n

- Statista (2013). *Ethylene Production Capacity Worldwide in 2013 by Region*. Available online at: <https://www.statista.com/statistics/270007/capacity-of-ethylene-by-region/> (accessed September 15, 2020)
- Sternberg, A., Jens, C. M., and Bardow, A. (2017). Life cycle assessment of CO<sub>2</sub>-based C1-chemicals. *Green Chem.* 19, 2244–2259. doi: 10.1039/c6gc02852g
- Stevenson, S. A. (2019). Thermodynamic considerations in CO<sub>2</sub> utilization. *AIChE J.* 65, 1–15. doi: 10.1002/aic.16695
- Turk, G. A., Cobb, T. B., Jankowski, D. J., Wolsky, A. M., and Sparrow, F. T. (1987). CO<sub>2</sub> transport: a new application of the assignment problem. *Energy* 12, 123–130. doi: 10.1016/0360-5442(87)90116-2
- Turton, R., Baile, R. C., Whiting, W. B., Shaeiwitz, J. A., and Bhattacharyya, D. (2015). *Analysis, Synthesis, and Design of Chemical Processes. 4th Edn.* Upper Saddle River, NJ: Pearson Education, Inc.
- US National Academy of Sciences (2019). *Gaseous Carbon Waste Streams Utilization: Status and Research Needs*. Washington, DC: The National Academies Press.
- von der Assen, N., and Bardow, A. (2014). Life cycle assessment of polyols for polyurethane production using CO<sub>2</sub> as feedstock: insights from an industrial case study. *Green Chem.* 16, 3272–3280. doi: 10.1039/C4GC00513A
- Wiesberg, I. L., de Medeiros, J. L., Alves, R. M. B., Coutinho, P. L. A., and Araújo, O. Q. F. (2016). Carbon dioxide management by chemical conversion to methanol: hydrogenation and bi-reforming. *Energy Convers. Manage.* 125, 320–335. doi: 10.1016/j.enconman.2016.04.041
- Wu, Q., Lin, Q. G., Wang, X. Z., and Zhai, M. Y. (2015). An inexact optimization model for planning regional carbon capture, transportation and storage systems under uncertainty. *Int. J. Greenh. Gas Control* 42, 615–628. doi: 10.1016/j.ijggc.2015.09.017
- Zhang, S., Liu, L., Zhang, L., Meng, Q., and Du, J. (2018). Optimal planning for regional carbon capture and storage systems under uncertainty. *Chem. Eng. Trans.* 70, 1207–1212. doi: 10.3303/CET1870202

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## GLOSSARY

### Acronyms

CCS	Carbon dioxide capture and storage
CCU	Carbon dioxide capture and utilization
CCUS	Carbon dioxide capture, utilization, and storage
DMC	Dimethylcarbonate
EOR	Enhanced oil recovery
EU	European Union
GHG	Greenhouse gas
MeOH	Methanol
MILP	Mixed integer linear programming
PPP	Polyether carbonate polyols
SC	Supply chain

### Sets

$g$	Region, $g = \{1, 2, \dots, 133, 134\}$
$k$	Capture option, $k = \{post_{coal}^{comb}, post_{gas}^{comb}, oxy_{coal}^{fuel}, pre^{comb}\}$
$l$	Transport mode, $l = \{pipeline, ship\}$
$\rho$	Transport capacity, $\rho = \{1, 2, \dots, 6, 7\}$
$\psi$	Chemical output, $\psi = \{PPP, MeOH\}$
$s$	Basin, $s = \{saline\ aquifer, gas\ field, coal\ field\}$

### Scalars

$A^\psi$	Scalar A for calculation of manufacturing cost of chemical $\psi$
$B^\psi$	Scalar B for calculation of manufacturing cost of chemical $\psi$
$C^\psi$	Scalar C for calculation of manufacturing cost of chemical $\psi$

### Parameters

$\alpha$	European carbon reduction target [%]
$CI_g$	Electricity carbon intensity in region $g$ [t/GJ]
$EEC_\psi$	Specific electric energy requirements for producing chemical $\psi$ [GJ/t]
$FC_\psi^{intercept}$	Array of intercept coefficients of the linearized facility capital cost for producing chemical $\psi$ [€]
$FC_\psi^{slope}$	Array of slope coefficients of the linearized facility capital cost for producing chemical $\psi$ [€/t]
$lab_{\psi,g}$	Labor cost for producing chemical $\psi$ in region $g$ [€/t]
$\dot{m}_{\zeta,\psi}$	Mass flowrate of output $\zeta$ for producing chemical $\psi$ [t/year]
$\eta_\psi^C$	Conversion efficiency of the process that generates chemical $\psi$ [t/t]
$\eta_\psi^R$	Amount of CO <sub>2</sub> that is needed to produce a unitary amount of chemical $\psi$ [t/t]
$P_{\zeta,g}$	Unitary price of commodity $\zeta$ for producing chemical $\psi$ [€/t]

$P_g^{max}$	Amount of anthropogenic CO <sub>2</sub> that is generated in region $g$ [t of CO <sub>2</sub> ]
$raw_{\psi,g}$	Unitary cost of raw materials for producing chemical $\psi$ in region $g$ [€/t]
$\hat{R}_{\psi,g}$	Unitary revenue from chemical $\psi$ in region $g$ [€/t]
$tax_g$	Taxation in region $g$
$util_{\psi,g}$	Unitary cost of utilities for producing chemical $\psi$ in region $g$ [€/t]
$U_{\psi,g}^{max}$	Productivity upper bound for chemical $\psi$ in region $g$ [t]
$U_\psi^{ref}$	Reference chemical plant capacity [t/year]

### Continuous Variables

$CF_{\psi,g}$	Cash flow from sale of chemical $\psi$ in region $g$ [€]
$COM_{\psi,g}$	Manufacturing cost for chemical $\psi$ in region $g$ [€]
$d_{\psi,g}$	Depreciation of chemical $\psi$ in region $g$ [€]
$FCI_{\psi,g}$	Fixed capital investment for producing chemical $\psi$ in region $g$ [€]
$profit$	Profit earned from sale of chemicals [€]
$R_{\psi,g}$	Revenue from sale of chemical $\psi$ (and by-products) in region $g$ [€]
$S$	Geologically sequestered CO <sub>2</sub> [t]
$TC$	Total cost [€]
$TCC$	Total capture cost [€]
$TSC$	Total sequestration cost [€]
$TTC$	Total transport cost [€]
$U_{\psi,g}$	Quantity of CO <sub>2</sub> sent to conversion process for producing chemical $\psi$ in region $g$ [t]
$U_{\psi,g}^{chem}$	Amount of chemical $\psi$ produced in region $g$ [t]
$U_{\psi,g}^{conv}$	Quantity of CO <sub>2</sub> converted and utilized for producing chemical $\psi$ in region $g$ [t]
$U^{conv}$	European converted CO <sub>2</sub> [t]
$U_{\psi,g}^{lost}$	Direct CO <sub>2</sub> emissions generated by conversion into chemical $\psi$ in region $g$ [t]
$U^{lost}$	European direct CO <sub>2</sub> emissions due to conversion facilities [t]
$U_g^{ind}$	Indirect CO <sub>2</sub> emissions generated by conversion processes in region $g$ [t]
$U^{ind}$	European indirect CO <sub>2</sub> emissions due to conversion facilities [t]
$U_{seq}$	European sequestered CO <sub>2</sub> [t]

### Binary Variables

$\delta_{\psi,g}^{chem}$	1 if chemical $\psi$ is produced in region $g$ , 0 otherwise
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