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# An overview of CO<sub>2</sub> capture and utilization in energy models

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## Abstract:

The recycling and utilization of CO<sub>2</sub> is gaining interest in the fight against global warming. Considering CO<sub>2</sub> not as a waste or a pollutant but as an opportunity is a concept that could prove promising for producing clean fuels in the future, as well as for producing chemicals, plastics and building materials. The extent of the benefits of Carbon Capture and Utilization (CCU) is still uncertain due to its many interactions with the rest of the energy system, and several energy models are trying to explore this area. As the global climate issue becomes an urgent policy priority, the scientific community is helping decision-makers choose the optimal technologies to successfully meet climate targets and decarbonize society. This paper reviews energy models that represent CCU as a decarbonization solution in an effort to understand and identify knowledge and modeling gaps. The results first show that CO<sub>2</sub> utilization is still poorly represented, and that when it is, it is rarely fully integrated. The conversion of CO<sub>2</sub> into fuels or chemicals is by far the most modeled of all the options CCU encompasses, while other key technologies for the decarbonization of the industry sector are barely considered. We discuss current CCU modeling methods and provide recommendations for future modelers who want to implement this set of technologies in their models. Additionally, we discuss the socio-economic drivers and barriers that could support or discourage the deployment of CCU in the future energy mix.

**Keywords:** CCU, CO<sub>2</sub> utilization, energy modeling, energy transition

## Highlights:

- We review energy models including CCU as a mitigation alternative.
- CCU is rarely considered in energy models, notably in global models.
- Energy models focus on the conversion of CO<sub>2</sub> into fuels and chemicals.
- Several recommendations are addressed to energy modelers seeking for modeling CCU.

## List of abbreviations:

BECCS	Bio-energy with Carbon Capture and Storage
BU	Bottom-up
CapEx	Capital Expenditure
CCS	Carbon Capture and Storage

CCU	Carbon Capture and Utilization
CCUS	Carbon Capture Utilization and Storage
CES	Constant Elasticity of Substitution
CGE	Computable General Equilibrium
CO <sub>2</sub>	Carbon dioxide
DAC	Direct Air Capture
EOR	Enhanced Oil Recovery
ESM	Energy System Model
ETP	Energy Technology Perspective
GDP	Gross Domestic Product
GHG	Greenhouse Gas
H <sub>2</sub>	Dihydrogen
IAM	Integrated Assessment Model
IEA	International Energy Agency
LCA	Life Cycle Assessment
MEA	Monoethanolamine
OpEx	Operational Expenditure
PSA	Pressure Swing Adsorption
PtG	Power-to-Gas
PtL	Power-to-Liquids
PZ	Piperazine
R&D	Research & Development
TD	Top-down
TEA	Techno-economic Assessment
TIMES	The Integrated MARKAL-EFOM System
TRL	Technology Readiness Level
VCM	Value Chain Model
VSA	Vacuum Swing Adsorption

## 1. Introduction

Global climate change and its consequences are threatening our societies due to our carbon-intensive lifestyles. In the future we will face water scarcity, starvation, ocean elevation, and biodiversity decline (IPCC, 2018), especially if we do not orient towards a decarbonized economy, hence the need to transition to clean energy sources. Under the Paris Agreement, to date, the European Union (European Commission, 2016), China (Climate Action Tracker, 2020), Japan (United Nations, 2020), South Korea (Gerresten, 2020) and New Zealand (Timperley, 2020), have declared their ambition to reach carbon neutrality by 2050, or 2060 for China. To achieve this goal, governments around the world are working to define and propose sustainable pathways through carbon neutrality, which can be determined and assessed by energy models.

Meeting climate commitments involves reducing emissions of current assets through energy efficiency, demand-side measures, emissions avoidance, and greenhouse gases (GHGs) removal. This picture is easy to draw but needs to be assessed in terms of economic implications, environmental impacts, and technical feasibility. Hence, the research community is working to investigate various

future pathways by designing energy models, such as Integrated Assessment Models (IAMs), representing the functioning of energy systems and the future transformations of energy supply when these systems are subject to a climate policy. The modeling community has been particularly prolific in recent years as, notably, it is now acknowledged that we should massively electrify our energy system and rely on negative emissions to offset the pollution we cannot abate easily (IEA, 2021; IPCC, 2018; Teske, 2019). Thereby, Carbon Capture and Storage (CCS) is determinant in delivering negative emissions, either through Direct Air Capture (DAC) (Fuss et al., 2018; Hanna et al., 2021; IPCC, 2018) or bioenergy with CCS (BECCS) (Fajardy et al., 2021; Köberle, 2019; Selosse, 2019). The capture of CO<sub>2</sub> can occur at many levels of an energy system, from energy extraction to power production, industry, and fuel generation. At all of these levels, CCS has been recognized as indispensable to reach our climate goals (Farell, 2018; IEA, 2019a; Morris et al., 2019).

It nevertheless remains uncertain how Carbon Capture and Utilization (CCU) will contribute to the global energy transition. Instead of storing CO<sub>2</sub> underground, the molecule can be utilized to manufacture fuels, chemicals, plastics and building materials (Alper and Yuksel Orhan, 2017; Aresta et al., 2013; Huang and Tan, 2014; Mustafa et al., 2020). Today, 200 Mt of CO<sub>2</sub> are employed for this purpose, more than a half of it to produce urea, used as a fertilizer (IEA, 2019b). Unfortunately, most of this CO<sub>2</sub> utilization results in CO<sub>2</sub> emissions when the CO<sub>2</sub>-based product is finally used. However, other niche CCU applications can avoid CO<sub>2</sub> emissions (Pérez-Fortes et al., 2016) and even deliver negative emissions (Hepburn et al., 2019). Moreover, CO<sub>2</sub> utilization is a way to enhance CO<sub>2</sub> that would have been captured either way, by transforming it into a valuable product. Given these two major considerations, CO<sub>2</sub> utilization can have a significant role in climate mitigation by bringing both economic and climate benefits.

Recent literature reviews show advances in carbon dioxide utilization (Ghiat and Al-Ansari, 2021) but also reveal three major barriers to its deployment: technology readiness (Ampelli et al., 2015; Mustafa et al., 2020), high energy consumption (Alper and Yuksel Orhan, 2017; Aresta et al., 2013; Huang and Tan, 2014) and high costs (Centi et al., 2020; Hepburn et al., 2019). Undoubtedly, these reviews gather information that can be extracted and implemented in energy models to represent a CCU chain and assess whether it can play a significant role in the future energy transition. Nevertheless, what energy models show about the contribution of CCU to climate change mitigation is neither clear nor subject to consensus. Indeed, the estimated potential of CO<sub>2</sub> captured and used globally varies from a few hundred megatons (IEA, 2019b, p. 2) to several gigatons (Kätelhön et al., 2019).

In view of the great variability of CCU's potential role in the future, it is unclear to what extent this set of technologies can help us mitigate climate change. Butnar et al. (2020) reviewed the role of CCU and CCS in the results of European energy models. They provide a detailed description of the potentials and mitigation impacts of CCU in European decarbonization scenarios and conclude that there is no clear future for CCU, either in terms of potential or role. They also argue that global energy models poorly represent CO<sub>2</sub> utilization. Another review reports the state-of-the-art of the programming tools and pinch analysis tools representing CCUS value chains, with a special focus on each branch of the value chain (Tapia et al., 2018). The authors also perform a bibliometric analysis of CCUS, revealing the growing interest for this set of technologies in the research community. This article mainly addresses operations planning of CCUS rather than assessing potentials and roles of CO<sub>2</sub> utilization through energy models and IAMs.

Although CCU is a major issue for the future, the modeling of this technology is limited in the literature. In an attempt to constitute a milestone for further modelings of CCU, the present paper describes the state-of-the-art of CO<sub>2</sub> utilization representation in energy models. The aim is to analyze shortcomings and trends in CCU modeling and to understand the results models provide on CO<sub>2</sub> utilization. We first discuss the motivations of modeling CO<sub>2</sub> utilization and analyze the trends in CCU modeling based on our literature review (section 2). Then we analyze how CCU is currently

modeled (section 3) before discussing the drivers of CCU and recommending best practices (section 4). We emphasize that this analysis does not focus on the results that the models return, but rather on how CCU is modeled.

## 2. Literature review of CO<sub>2</sub> utilization in energy models: motivations and trends

Energy modeling consists in representing the energy system of a geographic zone, which can be national, regional, or global. An energy system is defined as a close system guaranteeing satisfaction of energy demand through energy production, transformation, transport, and distribution. Usually, the purpose of energy modeling is to explore multiple pathways that policymakers should consider in order to tackle climate change or to reach energy policy targets e.g. related to energy security, resource scarcity, nuclear phase-out, etc. Modelers propose new paradigms for our society to produce and consume energy in respect of our energy-climate commitments and warn of the implications and requirements of such changes. Energy models comprise different structures (Böhringer and Rutherford, 2009) – bottom-up or top-down – and resolution methods (Helgesen, 2013) – optimization or simulation. Technologies such as CCU are key components of an energy model, as they behave as a means to transform energy and satisfy energy demand.

We searched the scientific literature for energy models that consider the capture and use of CO<sub>2</sub>. To do so, we browsed the *ScienceDirect* platform with keywords such as “CO<sub>2</sub> utilization, CO<sub>2</sub> conversion, energy models, modeling, CCU, Power-to-Gas and Power-to-Liquids” to find energy models taking into consideration at least one route that CO<sub>2</sub> utilization offers. We also looked at the IAMC platform (IAMC-Documentation contributors, 2021) and systematically reviewed each global model's presentation to see whether CCU was included as an option. The only selection criterion was that energy models should consider at least one CO<sub>2</sub> utilization route and provide sufficient detail to analyze the modeling. We examined each model in terms of:

- technology representation from capture to utilization in order to identify the origin of CO<sub>2</sub> (process CO<sub>2</sub>, fossil CO<sub>2</sub>, atmospheric CO<sub>2</sub> or biogenic CO<sub>2</sub>) and the final products made of CO<sub>2</sub>. We call “technology bricks” a stand-alone process producing an energy or material commodity such as a power plant or a CO<sub>2</sub> conversion process;
- modeling assumptions, i.e. the consideration of carbon taxes, techno-economic assumptions of CCU technologies, technology learning, etc.;
- model type, whether Energy System Models (ESMs) or Value Chain Models (VCMs) and bottom-up (BU) or top-down (TD) (Section 3);
- geographical perimeter;
- time horizon;
- climate target;
- the parametrization, i.e. the parameters used by the modelers in the study to characterize CCU.

Table 1 describes the 22 studies that have been reviewed. Currently, energy models rarely consider CCU as a decarbonization option (Butnar et al., 2020), yet their representation in energy models is vital for decision-makers to determine whether this technology set should be deployed extensively, as well as its role in mitigating climate and reducing the cost of carbon capture (Mac Dowell et al., 2017). Nonetheless, the few studies focusing on the use of CO<sub>2</sub> in energy models are mainly produced in the context of CO<sub>2</sub> emissions reduction, and particularly in the context of the Paris Agreement. Sometimes, CO<sub>2</sub> utilization is seen and modeled as a commercial opportunity (IEA, 2019b; Tapia et al., 2014), i.e. once CO<sub>2</sub> is captured it can be employed to produce goods, and this is the prime interest of modeling. Including CO<sub>2</sub> utilization as a novel option for energy models, researchers try to establish new paradigms, especially for the transport sector since the most targeted CO<sub>2</sub> utilization is

fuel manufacture. The authors' motive is to valorize the captured CO<sub>2</sub> rather than store it underground permanently. Thus, energy modeling seeks to determine the following key information:

- **The potential of CO<sub>2</sub> utilization**

Usually, the potential deployment of CO<sub>2</sub> utilization is expressed in terms of megatons of CO<sub>2</sub> utilized per year. It can also be evaluated by the quantity of CO<sub>2</sub>-based products supplying demand. For example, Blanco et al. (2018) explored under various policy scenarios the quantity of CO<sub>2</sub> to be converted into syngases to ensure European energy demand in the future.

- **The energy system transformation**

Utilizing CO<sub>2</sub> instead of venting is an appealing solution to mitigate climate change but can have strong impacts on the overall energy system, such as the required renewable power generation (Bazzanella and Ausfelder, 2017), the impact on land (Gabielli et al., 2020) and water scarcity (Dutta et al., 2017). This closely depends on the deployment rate of CO<sub>2</sub> utilization capacities to be installed: all of these impacts are linked and related to the quantity of CO<sub>2</sub> needed. Van Vliet et al. (2011) performed a complete study of the impact of alternative fuels (e-fuels included) on the transportation sector.

- **Environmental impact assessment**

Authors also explore the potential environmental impacts of CCU, such as pollutants and human health impacts. This kind of information is mostly determined through life-cycle assessments (Assen and Bardow, 2014; Cuéllar-Franca and Azapagic, 2015), and can also be evaluated by energy models.

- **Economic impact assessment**

Comprehending the impacts of CCU on the economy is crucial. Indeed, the transformation of the energy system is not just about CO<sub>2</sub> emissions reductions and environmental concerns; it also has collateral impacts on the economy, namely employment, fuel prices, electricity prices, consumption, and gross domestic product (GDP). These factors would condition whether a technology successfully enters the market, hence the importance of bringing this topic into the debate.

Ultimately, the purpose of modeling CO<sub>2</sub> utilization is to advise decision-makers on best practices to achieve energy transition by considering a number of side effects on other centers of interest such as environmental and socio-economic impacts.

Table 1: Overview of CCU modeling methods in energy modeling studies

Author	Context	Model name	Model type	BU vs TD	Region	Time horizon	Climate target	CO <sub>2</sub> capture	CO <sub>2</sub> utilization	Parametrization	Comments on the CCU modeling
(Fasihi et al., 2017)	The aim is to take advantage of the Maghreb's potential for solar and wind power generation to manufacture fuels with atmospheric CO <sub>2</sub> and green H <sub>2</sub> to satisfy European fuel demand.	Hourly Basis Model	Supply Chain	BU	Maghreb and Europe	2050	NZE emission	DAC	Power-to-Gas;Power-to-Liquids	CapEx and OpEx; Lifetime; Efficiencies; Other specific technical parameters	The capture of CO <sub>2</sub> is ensured only by DAC units fed with renewable electricity and heat. The utilization of CO <sub>2</sub> begins with its transformation into fuel products along with renewable hydrogen. The study provides two very detailed block-flow diagrams to represent the utilization units, production, storage, and delivery of syngas. The results rely on techno-economic assumptions that might be debatable for DAC.
(Farfan et al., 2019)	This study looks at capturing CO <sub>2</sub> emissions from cement plants to produce fuels and assesses the potential of CCU to mitigate cement factory emissions. The purpose is to estimate the quantity of CO <sub>2</sub> captured from the cement industry that could be used to make synthetic fuels.	N/A	Supply Chain	BU	World	2050	Different scenarios 1) Cement Sustainable Initiative target 2) 42.9% emissions reduction 3) Only process-related emissions remain	Cement plants	Power-to-Gas;Power-to-Liquids	Carbon capture efficiencies; Energy needs; Emissions levels per ton of cement; PTX energy and material flows	The authors simulate the potential of the cement industry in supplying CO <sub>2</sub> for fuel manufacture. Non-transparent modeling of CO <sub>2</sub> utilization with little techno-economic information about Power-to-X processes. The authors provide some references concerning the capture technologies, namely carbon looping and amine scrubbing.
(Kätelhön et al., 2019)	The idea is to assess the potential of CO <sub>2</sub> to replace hydrocarbon feedstocks for the chemical industry. The authors propose new paradigms for the chemical industry across three scenarios.	Technology Choice Model	Energy system	BU	World	2030	Decarbonization of the chemical industry	Industry;DAC	Power-to-Gas;Methanol; Olefins;Other chemicals	Energy consumption; Efficiencies; Environmental footprints;	This optimization is of a particular kind since it does not minimize the total annual cost, but rather the GHG emissions of the system. The CO <sub>2</sub> supply is ensured by high-purity industrial processes and DAC. Two main assumptions are made considering the carbon footprints of CCU plants involving a High-TRL scenario and a Low-TRL scenario. Technology data is summarized in open-access documentation, mainly from Ecoinvent and IHSdatabases.

(Bazzanella and Ausfelder, 2017)	This study analyzes how the European chemical industry could take advantage of new technologies to decarbonize its activity. The authors identify promising low-carbon technologies considering their potential impact on CO <sub>2</sub> emissions reduction, costs, technical performances and barriers.	No name	Energy system	BU	Europe	2050	Decarbonization of the chemical industry	Power plants;Industry	Urea;Methanol; Power-to-Gas;Power-to-Liquids;Plastics	Energy and material flows; Environmental impacts; CapEx and OpEx	The modeling of CCU is based on techno-economic parameters of processes with their related material and energy flows, as well as their environmental impacts. The added value of the study is that CCU routes are compared with alternative routes including electrification, biomass and recycling. Many efforts have been made to describe the new clean production systems the authors consider. The study includes sector-coupling with energy sector and the transport sector.
(IEA, 2019c)	Explores the implications of the unavailability of CO <sub>2</sub> storage on the energy sector, including the need for CO <sub>2</sub> utilization. Potential and opportunities are assessed in three different scenarios 1) Clean Technology Scenario (CTS) 2) Low Carbon Storage (LCS) and 3) Reference Technology Scenario (RCS). In the CTS and LCS, the focus is on the industry sector.	IEA Energy Technology Perspectives model	Energy system	BU	World	2060	75% cut in CO <sub>2</sub> emissions compared to 2017 levels	Industry;DAC;Power plants;Biomass;Hydrogen	Urea;Methanol; Concrete;Other chemicals;Plastics;Power-to-Gas;Power-to-Liquids	Energy and material flows; Environmental impacts; CapEx and OpEx	The IEA Energy Technology Perspectives (ETP) model depicts new opportunities for the energy system to shift from polluting production to clean production. This model is thus technology-oriented and yet poor assumptions are given about the economics of CCU processes. The modeling is based on the TIMES framework. The CO <sub>2</sub> tax is not applied to syngases made of biogenic CO <sub>2</sub> .
(Leonzio et al., 2020)	This study takes place in the context of a UK energy transition that aims to abate 6.4 Mton of CO <sub>2</sub> per year. The authors consider both storage and utilization and their related role in abating CO <sub>2</sub> emissions.	No name	Supply Chain	BU	UK	2030	6.4 MtCO <sub>2</sub> /yr emission reduction	MEA absorption ;PZ absorption	Methanol;Power-to-Gas;Polyurethane;Horticulture; Concrete;Calcium carbonate	Production costs; Capture costs; Material flows; Plants location	The specific constraints of CCU modeling are made explicit. For example, CO <sub>2</sub> cannot be sent to multiple storage sites, storage capacity is limited, minimum CO <sub>2</sub> abatement, etc. A detailed description of how the model works is provided. A carbon tax of 80 euros per ton is assumed.
(Leonzio et al., 2019)	A model is designed to assess the potential of carbon dioxide utilization and storage in Germany to satisfy methanol demand.	No name	Supply Chain	BU	Germany	2030	160 MtCO <sub>2</sub> /yr emission reduction	MEA absorption ;PZ absorption ;Membranes;PSA;VSA	Hydrogen;Methanol	Capture costs; Material flows; Plants location	
(Leonzio and Zondervan, 2020)	The model is designed to represent CCUS supply chains and define their framework to significantly reduce CO <sub>2</sub> emissions whilst minimizing total costs. The model is built for the Italian regions.	No name	Supply Chain	BU	Italy	2030	77 MtCO <sub>2</sub> /yr emission reduction	MEA absorption ;PZ absorption ;Membranes;PSA;VSA	Power-to-Gas	Capture costs; Material flows; Methane production costs; Plants location; Economic incentives for PtG processes	



(Blanco et al., 2018a)	The authors utilize a bottom-up model to evaluate the potential of methanation in the EU energy transition.	JRC-EU-TIMES	Energy system	BU	Europe	2050	80 to 95% CO <sub>2</sub> reduction by 2050 (vs. 1990)	Industry;DAC;Power plants;Biomass;Hydrogen	Power-to-Gas	CapEx and OpEx; Efficiencies; Availability; Lifespan; Energy and material flows	TIMES representation of technology bricks. No variable costs are represented as they are mainly supported by CO <sub>2</sub> feedstock of methanation processes. The modelers provide 3 different scenarios for PtG costs and 8 different policy scenarios of which two with no CO <sub>2</sub> storage available. A variable CO <sub>2</sub> price is considered.
(Blanco et al., 2018b)	The authors utilize a bottom-up model to evaluate the potential of PtL in the European energy transition.	JRC-EU-TIMES	Energy system	BU	Europe	2050	80 to 95% CO <sub>2</sub> reduction by 2050 (vs. 1990)	Industry;DAC;Power plants;Biomass;Hydrogen	Power-to-Liquids;Methanol	CapEx and OpEx; Efficiencies; Availability; Lifespan; Energy and material flows	TIMES representation of technology bricks with a high level of detail (23 processes). The modelers provide different scenarios for PtL costs. A variable CO <sub>2</sub> price is considered.
(Dutta et al., 2017)	The proposed model is employed to assess the contribution of CO <sub>2</sub> utilization to produce power and chemicals. Instead of minimizing the total cost, they maximize CO <sub>2</sub> avoidance. Three scenarios considering different renewable H <sub>2</sub> availability are studied.	No name	Energy system	BU	World	Not stated	1 to 59% CO <sub>2</sub> emissions reduction compared to 2013 level	N/A	Hydrogen;DME;Methanol;Olefins;Urea	Environmental impacts	The model is fed with CO <sub>2</sub> avoidance inputs that reflect the CO <sub>2</sub> that would not be emitted into the atmosphere if the alternative CCU option were chosen by the model. The total amount of CO <sub>2</sub> avoided resulting from the optimization is evaluated considering the CO <sub>2</sub> emission factors of remaining fuels. Three scenarios are discussed including with unlimited renewable hydrogen. Costs are not considered since the objective function is to maximize CO <sub>2</sub> avoidance.
(Williams et al., 2021)	The United States is supposed to reach carbon neutrality by mid-century following IPCC recommendations. Two models are developed and utilized to model the entire US and industrial system. One is capable of making technology choices at the demand-side level. The other addresses the sequential hourly variation of renewable energy over a sampling of representative days to find the lowest cost solution to decarbonize energy supply.	EnergyPATH WAYS & RIO	Energy system	BU	USA	2050	Decarbonation target	Industry;DAC;Biomass	Power-to-Liquids;Power-to-Gas	CapEx and OpEx; Efficiencies; Availability; Lifespan; Energy and material flows	The modeling of CCU is achieved in a typical BU fashion. It comprises the capture of CO <sub>2</sub> from highly concentrated streams in industry or biogenic CO <sub>2</sub> directly from air or biomass conversion. Then CO <sub>2</sub> is utilized for a single purpose, i.e., to manufacture fuels as energy carriers or feedstocks (e.g. for the chemical industry). In most scenarios, the captured CO <sub>2</sub> is biogenic, so the majority of manufactured fuels are climate-neutral.
(Tapia et al., 2014)	First-of-a-kind study working on the optimal design and planning of a CCUS value chain that only considers EOR as a CO <sub>2</sub> utilization option.	No name	Supply Chain	BU	N/A	Not stated	No stated target	N/A	EOR	OpEx; Lifespan	The authors run an optimization model maximizing the profit that can be generated from EOR and provide a description of its basic framework. Data about operation costs are included. The study focuses on the end-of-the-pipe, meaning that only utilization is considered and not capture.
(Teske, 2019)	Global complete energy transition pathways at different regional scales for a decarbonized world in 2050.	Global GHG model +TRAEM + Energy System Model + [R]E 24/7	Energy system	Hybrid	World	2100	Decarbonization target	Biomass	Power-to-Liquids	CapEx; Efficiencies	The modeling methodology of CCU is described simply but the interaction between the capture of CO <sub>2</sub> , the utilization and the combination with hydrogen is not explicit.

(Khalili et al., 2019)	Exploration of scenarios for the transportation sector in the context of the Paris Agreement. The aim is to study the penetration of new options in the transportation sector to reach 100% renewable by 2050.	No name	Energy system	Hybrid	World	2050	Decarbonization target	N/A	Power-to-Liquids;Power-to-Gas	CapEx and OpEx; Efficiencies; Availability; Lifespan	The modeling of the transport sector is very concise and identifies great potential for rail, marine and aviation sectors to be decarbonized through syngas, while road transport is more likely to be decarbonized by electric and hydrogen cars. The modeling of new opportunities is mainly achieved by feeding the model with new processes and their related costs, efficiencies and environmental impacts.
(Bogdanov et al., 2019)	Modeling of the energy sector and its interactions with the transport sector and industry to capture the interest of sector coupling to reach a climate-neutral European energy system. Capture technologies are not allowed for the power sector but Power-to-X solutions can be addressed for the transport sector with atmospheric CO <sub>2</sub> .	LUT Energy System Transition Model	Energy system	BU	World	2050	Decarbonization target	DAC	Power-to-Gas;Power-to-Liquids	CapEx and OpEx; Lifespan; Energy and material flows; Efficiencies; Learning rates	The model includes many Power-to-X possibilities in which the CO <sub>2</sub> supply is systematically ensured by cheap DAC processes with a CapEx below 200 \$/t. The choices in PtX pathways are mostly driven by techno-economic inputs. The authors also state that minimum and maximum capacity limits are given into the model so that the penetration of such technologies remains feasible. A detailed description of techno-economic assumptions is provided in Supplementary Information.
(Capros et al., 2019)	Power-to-X routes are introduced into a European energy model to propose sustainable optimal profiles of energy supply in a climate-neutral energy system.	PRIMES	Energy system	BU	Europe	2070	80% emission cut compared to 1990 or climate neutrality	DAC;Power sector;Industry;Biomass	Power-to-Gas;Power-to-Liquids;Other chemicals	CO <sub>2</sub> emissions from energy and processes; Production costs	In order to ensure the climate benefit of Power-to-X solutions, the authors only consider a non-fossil origin for CO <sub>2</sub> , but the model also considers CO <sub>2</sub> capture for the power sector. Additionally, dihydrogen molecules feeding these processes come from carbon-neutral electricity. Synthetic fuels are available only for road transport and compete with at least 8 other fuel types, which restricts the potential PtX roll-out.
(Siskos et al., 2015)	A technology-rich model running over endogenous demand is utilized to propose a decarbonization strategy solely for the European transport sector, in which Power-to-X solutions are made available within the model.	PRIMES-TREMOVE	Energy system	Hybrid	Europe	2050	Decarbonization	DAC;Power sector;Industry;Biomass	Power-to-Gas;Power-to-Liquids;Other chemicals	CES functions; CO <sub>2</sub> emissions from energy and processes; Production costs	The PRIMES-TREMOVE model is an extension of the PRIMES model devised to generate endogenous energy demand profiles. The modeling is thus composed of two dynamic steps 1) a technology choice module determining the vehicle technologies with their related fuels as a result of a discrete problem based on technology costs 2) a transport demand module simulating the demand for transport considering the transport activity and the maximized passenger utility. CES functions are utilized to describe the technologies and fuel choices of consumers.
(Takeshita, 2013)	Global assessment of CO <sub>2</sub> capture and storage in a cost-optimal fashion. The authors include one technology to convert pure CO <sub>2</sub> into methanol for industrial thermal demand.	REDGEM70	Energy system	BU	World	2050	50% cut in CO <sub>2</sub> emissions compared to 2005 level	Power plants;Biomass;Fischer-Tropsch process	Methanol	Techno-economic attributes; Emissions reductions	The authors perform a cost-optimal scenario with price-induced energy demand reductions and fuel switching, notably CO <sub>2</sub> utilization is not at the core of the study but is part of a rich description of the supply chain in a bottom-up fashion, enabling sector coupling studies.
(Quarton and Samsatli, 2020)	In the context of growing interest in CCS and CCU technologies, the authors take into consideration this set of technologies to decarbonize the British energy system.	Value Web Model	Energy system	BU	UK	2050	Decarbonization target	Power plants;Hydrogen	Methanol	Techno-economic parameters; Demands; Existing capacities;	The authors provide a transparent mathematical description of the model formulation for CO <sub>2</sub> utilization technologies with the total rate of CO <sub>2</sub> production from industrial emissions, economic penalties, and rewards for CCUS processes. Economic incentives for CCUS are modeled, i.e., CO <sub>2</sub> pricing and variation of methanol market price.

(Cunha et al., 2020)	No particular study on CO <sub>2</sub> utilization has been performed with this model, to our knowledge. But the model still represents EOR as an option to produce liquid fuels.	COFFEA-TEA	Energy system	TD	World	2100	N/A	Power plants;Hydrogen;Industry	EOR	Carbon storage coefficient; CO <sub>2</sub> injection rate per barrel; Production costs	The model makes a distinction between EOR storage fields and saline aquifers. The potential for CO <sub>2</sub> storage is calculated from the amount of oil that can be recovered with CO <sub>2</sub> injection, considering a coefficient varying between 0.27 and 0.32 tCO <sub>2</sub> per barrel.
(Zhang et al., 2020)	In order to deploy CCUS or mitigate CO <sub>2</sub> emissions, the authors design the best utilization framework. The models are solved both by cost minimizing and emission minimizing.	No name	Supply Chain	BU	North-East China	Not stated	70 MtCO <sub>2</sub> /yr emissions reduction	Power plants;Industry;Bio mass	EOR	Dehydration costs;Capture costs;Pipeline transportation costs;Injection costs; Revenue from EOR;Emission factors from LCA; CO <sub>2</sub> sources; CO <sub>2</sub> reservoirs	Very detailed mathematical assumptions are provided regarding the CO <sub>2</sub> sources to be selected for capture, the pattern for CO <sub>2</sub> pipeline transportation, CO <sub>2</sub> capture technology, utilization and storage nodes, and optimal cost-based deployment strategy of CCUS supply chains.

Simply registering the number of occurrences for a specific utilization process, we notice that CO<sub>2</sub>-to-fuels processes stand out from the crowd (Figure 1), followed by CO<sub>2</sub>-to-chemicals processes. “CO<sub>2</sub>-to-fuels” is a generic term to qualify technologies that process CO<sub>2</sub> and H<sub>2</sub> to manufacture either liquid (PtL) or gaseous (PtG) fuels ultimately meant to be burned. Sometimes, the term PtG is used to define the conversion of renewable electricity into hydrogen through electrolysis. Here, PtG refers solely to the manufacture of synthetic natural gas or methane. When hydrogen features as an output of CO<sub>2</sub> utilization in Figure 1, this means that the authors are considering the dry reforming of methane (Carapellucci and Giordano, 2020). PtL includes diesel, gasoline, and jet fuels.

In Figure 1, the “chemicals” label comprises methanol (which can both be considered as a fuel and a feedstock for the chemical industry), along with olefins, formic acid, ethanol, dimethyl carbonate, acetic acid, and ethylene carbonate. Urea is a particular product that is often represented in integrated assessment models because it is currently the largest consumer of CO<sub>2</sub> and its production is expected to continue because of population growth. Thus, due to its current status, CO<sub>2</sub>-to-fertilizers needs to be represented in models to better represent the potential of CO<sub>2</sub> capture. However, this utilization does not constitute an option for CO<sub>2</sub> emissions mitigation, unless biogenic or atmospheric CO<sub>2</sub> is used. Contrary to fuels, chemicals, and fertilizers, much less attention is paid to building materials, plastics and biomass growing despite the fact that these CO<sub>2</sub> uses will certainly bind CO<sub>2</sub> for longer periods, thus having a positive impact on the climate.

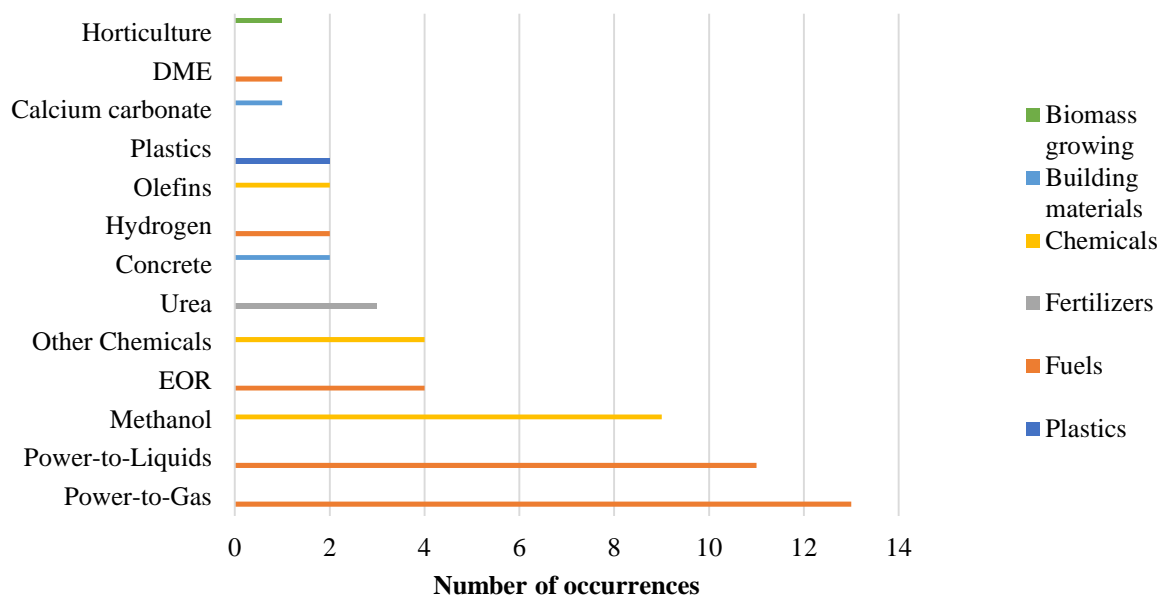


Figure 1: Occurrences of specific CO<sub>2</sub> utilization bricks over the 22 models reviewed

Energy models tend to focus on the potential of only one CO<sub>2</sub>-to-X option. Energy models that include various CCU options (Bazzanella and Ausfelder, 2017; Leonzio et al., 2020) are rarely performed. Consequently, it is currently difficult to envision the real potential of CO<sub>2</sub> utilization in the future through energy models. Other studies that do not employ energy models still identify CO<sub>2</sub>-to-fuels and CO<sub>2</sub>-to-chemicals as the most interesting options in the CO<sub>2</sub> utilization package (Armstrong and Styring, 2015; “CO<sub>2</sub> Utilization,” 2017; Gabrielli et al., 2020; Hepburn et al., 2019; ICEF, 2016). Thus, the domination of CO<sub>2</sub>-to-fuels and CO<sub>2</sub>-to-chemicals representation in energy models is in line with the expectations of studies of a different kind. This also corresponds to the funding attributed to CO<sub>2</sub> utilization in R&D (Kapetaki et al., 2019) in favor of CO<sub>2</sub>-to-fuels and CO<sub>2</sub>-to-chemicals.

### 3. How CO<sub>2</sub> utilization technologies are represented in energy models

Since the place of CCU in the results of energy models is highly dependent on how it is modeled, we review the assumptions and methods of the models in the present section. As indicated in the fourth column of Table 1, two types of model can be differentiated. On the one hand, Energy System Models (ESMs) focus on modeling the energy system by considering several options for decarbonization. Therefore, CCU is just one of the options available to ESMs to mitigate climate change and these models need to represent different value chains to capture the competition between each other and deliver a realistic assessment of future needs. Thus, in the chemical sector, one study for example considered biomass energy and renewables in addition to the use of CO<sub>2</sub> in order to better capture both interactions and competition between them (Bazzanella and Ausfelder, 2017). In the transport sector, Blanco et al. (2018a) also took into account biofuels, electricity, and hydrogen. This kind of model is useful to evaluate the change in energy production assets considering several value chains in terms of their potential and contribution to reach a climate target. On the other hand, Value Chain Models (VCMs) focus on the specific chain of CCU – or CCUS – from the capture site to the utilization site, comprising transport and the many other processes involved. This ensures a detailed and comprehensive representation of CCU and may capture information that ESMs cannot grasp in terms of technology feasibility and details (Fasihi et al., 2019) as well as geographical constraints and technology insertion into the geographic scope of the current energy system (Leonzio et al., 2020, 2019; Leonzio and Zondervan, 2020; Zhang et al., 2020). Generally, the purpose of VCMs is to design optimal supply chains of carbon in order to satisfy an industrial demand under the climate constraint. They can determine and quantify the least costly CO<sub>2</sub> emission point sources, capture technologies, transportation design, and fate of CO<sub>2</sub> (whether storage or utilization).

Thus the main difference between ESMs and VCMs lies in the level of aggregation of a technology. Generally, ESMs are utilized in prospective studies attempting to forecast a sustainable path to reach energy system decarbonation. Consequently, these models are time dynamic, i.e. they solve multi-period problems based on optimized solutions, and need to parametrize CCU mainly with techno-economic and environmental performances (see the last two columns of Table 1). Contrarily, VCMs do not usually deliver results over time, but propose a new static way of including CCU in the current energy mix to mitigate a determined quantity of carbon. They often need to parametrize their modeling with geographical data on the location of capture, utilization and storage sites. From our overview, 15 ESMs integrate the use of CO<sub>2</sub> as a lever to reach a climate target, in competition with other alternatives such as hydrogen, biomass and electrification (Table 1). The remaining 7 models are VCMs.

To be more specific, the ESM family includes two members, namely bottom-up (BU) and top-down models (TD), that are distinguished by the way they integrate and represent the energy sector (Figure 2). Table 1 indicates in the fifth column whether the model is BU or TD.

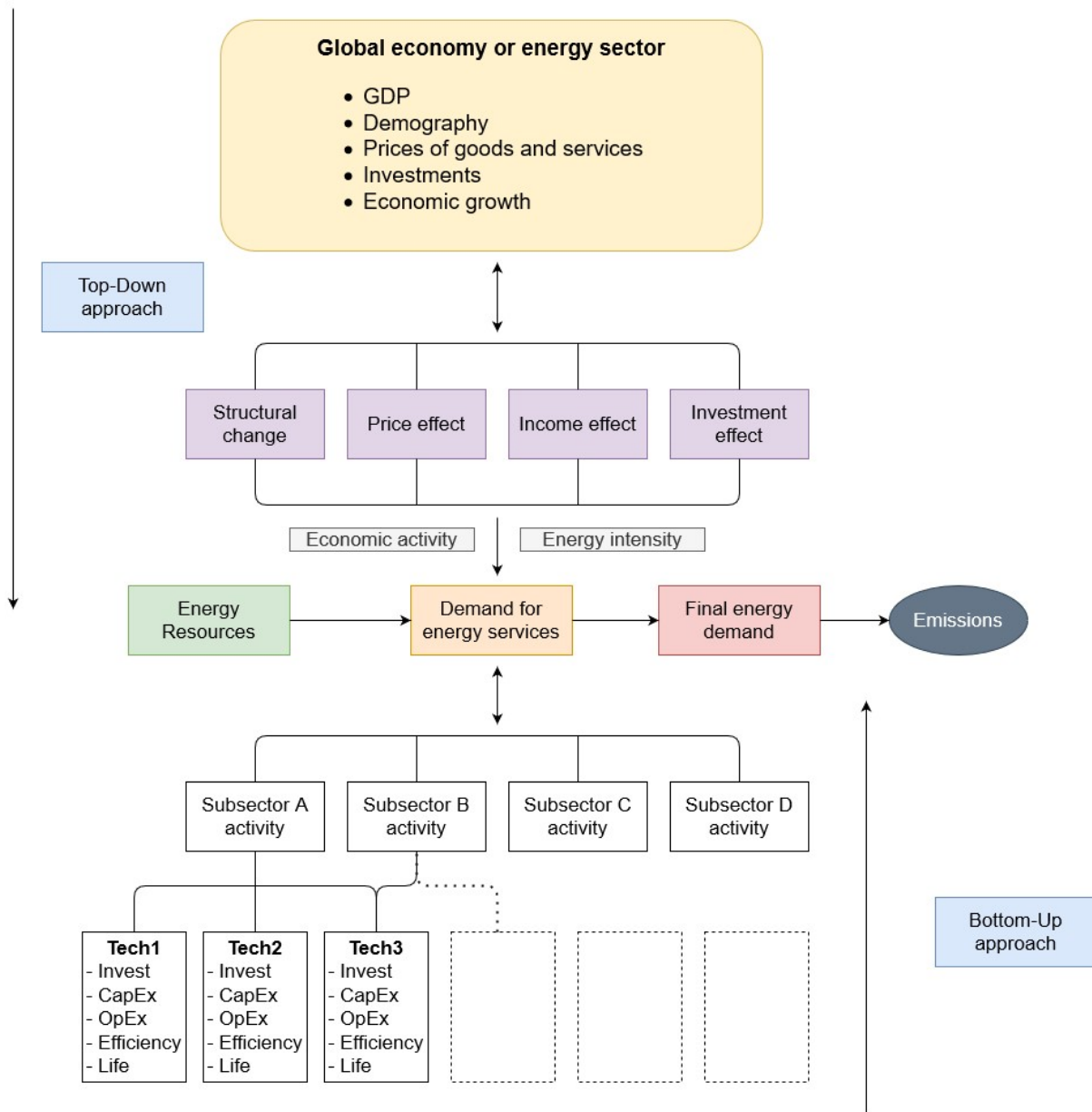


Figure 2: Diagram of bottom-up and top-down approaches inspired by (Assoumou, 2006)

BU models are characterized by their high level of technological detail (Assoumou et al., 2018; Subramanian et al., 2020). The models' rich representation of the energy system enables the modelers to describe any process in a complete way, including energy, material and pollutant flows, and the economic and financial properties related to an investment, including capital costs, operation costs, lifetime, discount rate, etc. (Sathaye and Sanstad, 2004). These data are most often extracted from existing techno-economic studies (Algehed et al., 2009), which explains the high diversity of inputs from one model to another. Such a need for an extensive database constitutes a major drawback for BU models (Subramanian et al., 2020). Figure 3 gives a generic example of what a CCU supply chain resembles in BU models, as one can find in the BU references in Table 1.

BU models mainly try to determine an optimal framework that minimizes the total annual cost of fulfilling energy demand or maximizing energy efficiency by selecting the appropriate technologies under several constraints, e.g. potentials and availability of resources, carbon tax, or GHG emissions limited to an upper bound. The results vary from one model to another depending on the level of

temporal, spatial, technical and economic detail, as well as their ability to consider sector coupling (Prina et al., 2020). They are mainly addressed at industrial and non-industrial policymakers in search of robust strategic planning of energy generation in respect of climate goals. Nevertheless, BU models are criticized for providing results with poor behavioral and economic realism (Hourcade et al., 2006). Since they only model the evolution of an energy system over time, they are unable to assess the future demand for energy services across sectors, which is highly dependent on interactions with the rest of the economy. Therefore, these models need to be fed with exogenous energy demand forecasts (Helgesen, 2013) which can be imported from TD models (Loulou and Labriet, 2008). TIMES models are good examples of BU models (ETSAP, 2021) (Table 1).

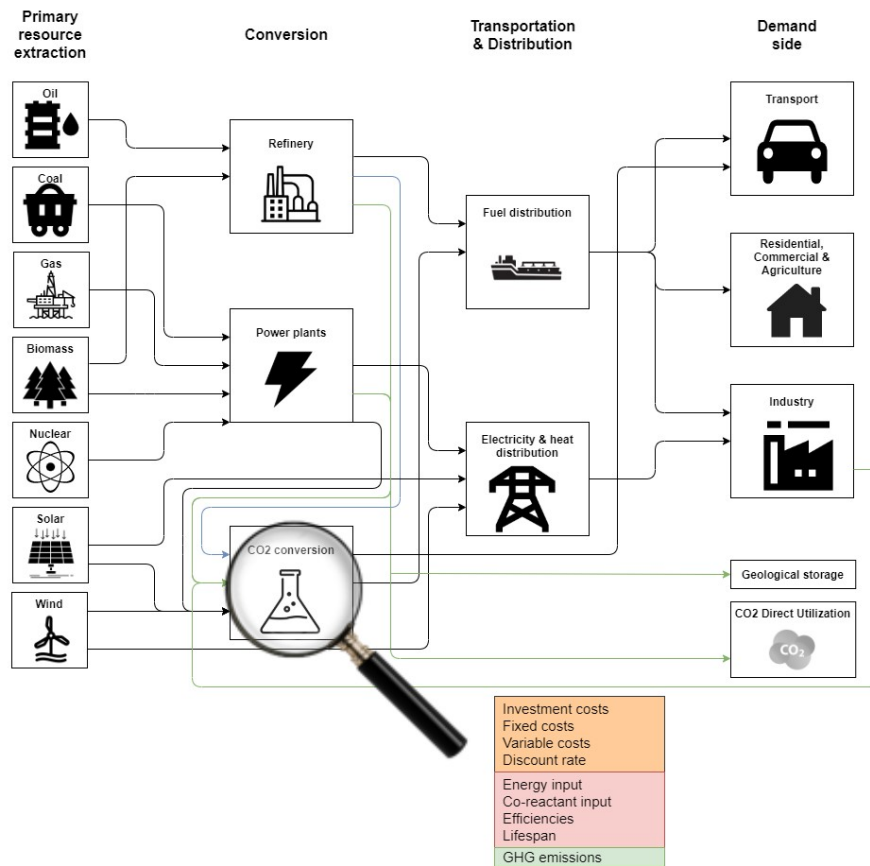


Figure 3: CCU generic modeling under BU frame inspired by (Subramanian et al., 2020)

One characteristic of BU models is that they consider a large array of techno-economic properties and constraints for any technology bricks or processes, which are here embodied in the rectangles and squares. These include pure economic ones (orange box), technical ones (red box) and environmental ones (green box)

Indeed, TD models are based on the interactions between the energy system and the rest of the economy, notably through econometric techniques and Computable General Equilibrium (CGE), since they model all sectors of the economy. They are known to give a broad representation of the entire economy at the expense of low technology explicitness (Assoumou et al., 2018), i.e. available technologies are often aggregated into technology packages with few details on how the process works and neglecting sector coupling (Prina et al., 2020). Typically, the coal power sector is embodied in one process, whilst BU models feature different processes for coal power generation, including supercritical pulverized coal, atmospheric fluidized bed, and others. However, their strength is that they can capture feedback from markets by representing primary production factors and consumption of goods considering prices, incomes, and savings. Thus, TD models perform a general equilibrium of the entire economy while BU models perform a partial equilibrium of the energy sector. One branch of TD models is called CGE, which operate on the basis of microeconomics (Assoumou et al., 2018; Hourcade et al., 2006) through social accounting matrixes, elasticities of

various kinds and Constant Elasticities of Substitution (CES) functions (Algehed et al., 2009). Governments and economists utilize this family of models to assess the impact of an energy policy on the rest of the economy. Figure 4 shows a generic simplified diagram of how CO<sub>2</sub> utilization can be incorporated into a CGE model.

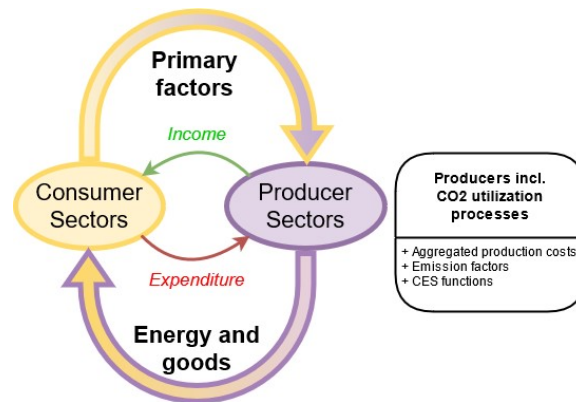


Figure 4: CCU generic modeling in TD models

*In TD models, techno-economic properties of the processes composing the energy sector or the producer sector are not diverse but mostly aggregated and require other information such as CES functions (represented in the side box). In exchange, TD models focus better on modeling the economic feedback that consumers return to producers (represented by the top arrow)*

Behind the CES functions of CGE models are price elasticities and elasticities of substitution that reflect the preferences and willingness of consumers to switch from one way of consuming to another (Chen et al., 2017, p. 5; Rutherford, 2009). These elasticities are nested to form a cost function with multi-level nodes representative of the consumer’s behavior for a utility. For instance, synfuels can be included in a CGE model as in Figure 5 with the PRIMES-TREMOVE model (Capros and Siskos, 2011). In this decision tree representing small cars, the consumer faces a first choice between a vehicle running on gasoline, diesel, pure electric or hydrogen, then a second choice for the refueling type, and a last choice for a fuel input whose carbon content is dependent on European norms (ACEA, 2021). Thus, if production costs and prices relative to synfuels are implemented upstream, we might imagine alternative CO<sub>2</sub>-based fuels to be included in one of the European classifications.

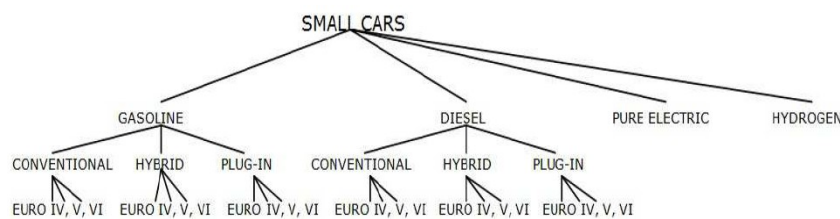


Figure 5: CES function for small cars in the PRIMES-TREMOVE model (Capros and Siskos, 2011)

Thus, ESM can either be classified as BU or TD, depending on the aggregation level of the technology.

Some models combine both BU and TD characteristics and are classified as hybrid (Helgesen, 2013; Hourcade et al., 2006). As Table 1 shows, we note a clear domination of BU models in the modeling of CO<sub>2</sub> utilization. This may be symptomatic of the lack of socio-economic data related to CCU that TD models require.

Nevertheless, important data about the techno-economic and environmental performances of CO<sub>2</sub> utilization processes can be found in the references of Table 1. This information determines input commodities (e.g., electricity, hydrogen and CO<sub>2</sub>) to deliver output commodities (e.g. synfuel, chemicals, etc.) considering a specific CapEx, OpEx and efficiency (Figure 3). The origin of CO<sub>2</sub> is of



great interest because it reflects the purpose of CO<sub>2</sub> utilization and leads to a more comprehensive analysis of the contribution of CCU in decarbonizing energy systems:

- If the CO<sub>2</sub> is biosourced or captured from the atmosphere, then the processes transforming or directly utilizing CO<sub>2</sub> can generate negative emissions or carbon-neutral products, depending on the CO<sub>2</sub>-based product generated. The previous statement is true in theory, but in practice biomass management and DAC can generate emissions at many levels of the CCU chain, which would make the overall CCU process a net emitter (Cuéllar-Franca et al., 2019);
- If the CO<sub>2</sub> comes from industrial emissions, then CO<sub>2</sub> utilization processes can leverage the cost of capturing unavoidable CO<sub>2</sub> from the industry by adding value to it, rather than storing it more expensively.
- If CO<sub>2</sub> is emitted due to the combustion of fossil resources and treated afterwards, this can be helpful to guarantee a degree of flexibility on the electricity network. Energy-related CO<sub>2</sub> is cheaper to capture than to process, and cheaper than biogenic CO<sub>2</sub>, so it can be an opportunity to run CO<sub>2</sub> utilization processes at the lowest cost.

As Figure 6 shows, biogenic and atmospheric CO<sub>2</sub> utilization are of great interest concerning the production of CO<sub>2</sub>-based products or the direct utilization of CO<sub>2</sub>. Indeed, treating biogenic CO<sub>2</sub> is essential to ensure that CO<sub>2</sub> utilization processes have a beneficial or neutral impact on climate due to the short lifespan of CO<sub>2</sub>-based products. As most of the studies discuss the contribution of synfuels in climate mitigation (Figure 1), modeling climate neutral CO<sub>2</sub> capture is a milestone and explains why so many of them feature DAC and bioenergy with carbon capture processes. In some studies, in fact, biogenic CO<sub>2</sub> is the only available option for CO<sub>2</sub> utilization processes (Bogdanov et al., 2019; Fasihi et al., 2017), and is not subject to the carbon tax (IEA, 2019c). Carbon capture for the hydrogen industry does not seem to be of interest in CCU modeling, although it is one of the cheapest options for carbon capture processes (Leeson et al., 2017). In the power sector, carbon capture is generally modeled because it is a common mean to decarbonize power generation, and consequently electrolysis. The literature on techno-economic assessments of carbon capture processes has been very prolific in recent years, so that it is now commonly present in models, with different levels of detail: BU models can consider diverse post-combustion CO<sub>2</sub> reactants (e.g. MEA, PZ, membranes, etc.) and include pre-combustion and oxycombustion capture techniques as well. Their modeling is not necessarily designed to feed CO<sub>2</sub> utilization facilities, but rather to generate negative emissions through BECCS, or simply to help decarbonize electricity generation.

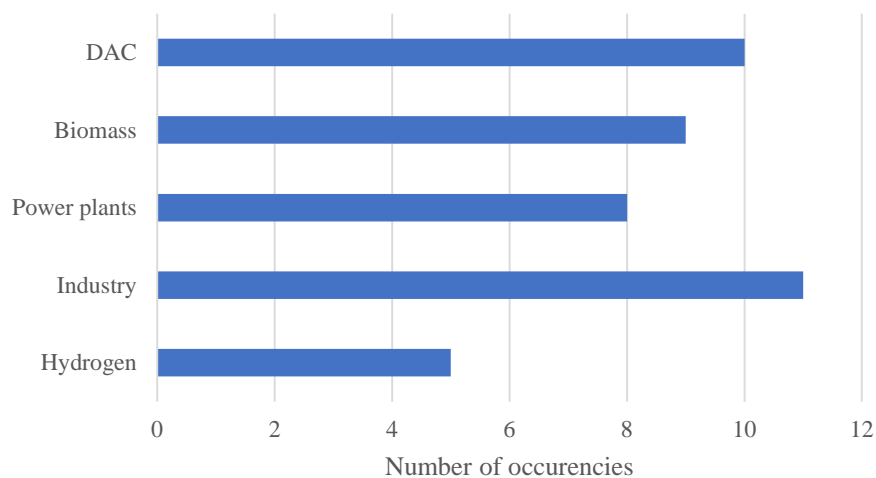


Figure 6: Occurrence of capture means in the 22 models of the review

Thus, depending on the model, CO<sub>2</sub> capture is found at different levels of the energy system. However, we note that modeling capture at all levels is a rare but crucial practice to fully integrate the CCU chain in the models, and thus better assess its potential.

## **4. Discussion, recommendations, and drivers of CCU**

### **4.1. Barriers to including CCU in energy models**

The previous sections have highlighted that, according to the set of models reviewed, the modeling of CCU suffers from four major flaws, namely: a lack of integration for capture processes; a lack of consideration of the various utilization routes notably for the industry sector; a lack of modeling at the global level; and a lack of modeling in TD models. We can see an obvious reason why CCU is poorly modeled, and that is the lack of data. The past five years have been quite prolific with regard to the number of TEA and LCA studies about the conversion of CO<sub>2</sub> into fuels and chemicals (Marchese et al., 2021), but other options for utilizing CO<sub>2</sub> tend to be neglected. As a matter of fact, the TEAs and LCAs reveal that the major techno-economic barriers that CCU faces are low TRL (Chauvy et al., 2019), low development potential (Ampelli et al., 2015), high costs of CO<sub>2</sub> capture (Fuss et al., 2018; Irlam, 2017; Leeson et al., 2017), and limited climate benefits (Ravikumar et al., 2021).

The number and importance of these barriers may discourage modelers from implementing the CCU option within their models. At least these barriers have the benefit of being quantitative and easy to model, but other hard-to-model barriers related to energy markets and the economy work against the integration of CCU in energy models. Indeed, the current demand for CO<sub>2</sub>-based products (mainly fertilizers at the moment) is still low (Kapetaki et al., 2019, sec. 5.3.2) and not expected to grow substantially unless synfuels emerge and benefit from their high substitutability with current products. However, CO<sub>2</sub>-based products are currently too expensive compared to conventional processes and cost-competitiveness is an acknowledged key challenge to be addressed. To date, EOR is the only CO<sub>2</sub> utilization process that can compete with conventional processes (Hepburn et al., 2019), thus stakeholders have no interest in investing in other CCU options for now. Competition also occurs between other equally useful low-carbon options for decarbonizing the various sectors of an energy system. In general, energy models choose the cheapest technology to satisfy energy demand as they usually perform a cost minimization. Given the wide pallet of possibilities, CCU options are thus not likely to rank high in the merit order. Finally, chemical and fuel markets are difficult to penetrate because they are already saturated, capital-intensive and highly competitive (de Pee et al., 2018). As a result, we find it difficult to imagine new players entering the market with products manufactured *via* CCU. It is much more likely that incumbent stakeholders would retrofit their existing assets with CCU. This requires that energy models consider existing agents separately from potential new agents in their representations, which is not a common feature of such models.

Thus, we assume that CCU suffers from a lack of consideration in energy models because of the many aforementioned hurdles. In addition to these obstacles, it is essential to state that CCU might not be beneficial to the climate issue, notably because most CO<sub>2</sub>-based products cannot retain carbon for long periods of time. As we highlighted in the previous section, CO<sub>2</sub> utilization processes running on non-fossil CO<sub>2</sub> (i.e. atmospheric or biogenic) would likely be favored in the future as they can be carbon negative or carbon neutral, in theory. In reality, producing concentrated climate-neutral CO<sub>2</sub> is currently expensive and technically difficult to achieve because it relies on many processes which themselves emit CO<sub>2</sub>. Taking the example of biogenic CO<sub>2</sub>, we see that forest management, transport of biomass feedstock, the biomass feedstock process, and capture of CO<sub>2</sub> can, in the end, be detrimental to the overall CCU process and make it a net CO<sub>2</sub> emitter. Additionally, the period of time during which the forest regrowth reabsorbs atmospheric CO<sub>2</sub> emissions far exceeds the CO<sub>2</sub> emissions from biomass combustion, thus having the opposite effect of what is called 'renewable energy' – this is mainly true for woody biomass and less so for energy crops. Hence, biomass carbon neutrality, as

generally assumed in models and calculations, has increasingly been demonstrated as incorrect and misleading (Norton et al., 2019; Slade et al., 2018). Consequently, caution should be exercised when modeling biogenic CO<sub>2</sub>.

In the face all of these barriers and uncertainties, there are apparently good reasons not to consider CCU in energy models. However, interest in CCU modeling should not stop with these seemingly unfavorable characteristics because they can be consolidated or refuted by energy models. Moreover, both industrialists and individuals are much more interested in CCU than in CCS, with regard to the number of global CCUS projects (IOGP, 2021), because the former generates revenues while the latter only involves costs if the carbon prices rise enough. Regarding industrialists' interest in CCU, energy models could be used, not to estimate CCU potentials, but to assess the climate impacts of CCU if stakeholders commit to developing this technology. Thereby, we strongly call for the modeling of CCU.

#### **4.2. Drivers of CCU in energy models**

Interestingly, the aforementioned barriers can be mitigated or counterbalanced with other measures or breakthroughs to be implemented in energy models. Because of the many interactions that link CO<sub>2</sub> capture and utilization to the rest of the energy system, there are several parameters adjacent to CCU that are nevertheless part of its modeling and that can influence the results of energy models, namely the hydrogen sector, the electricity sector, and various demand sectors.

Firstly, low-carbon electricity is both a competitor and a promoting agent for CO<sub>2</sub> utilization because a large part of CO<sub>2</sub>-based products can be manufactured through electrochemical conversion processes that are cost-driven by electricity. Feeding CCU processes with dedicated low-carbon electricity generation is thus a lever that would ensure the implementation of processes to avoid CO<sub>2</sub> emissions rather than conventional processes. It would attract a great deal of interest if this low-carbon electricity were generated at costs lower than 50 USD/MWh (de Pee et al., 2018). Likewise, hydrogen is both a competitor and co-reactant of most CO<sub>2</sub> utilization processes. As a result, clean, cheap production of hydrogen is an important milestone for CCU deployment. To illustrate the importance of this lever, one study explored the potential of CO<sub>2</sub>-based products when the availability of renewable hydrogen varies and confirmed that the potential for CO<sub>2</sub>-to-fuels is way greater when renewable H<sub>2</sub> is an unlimited resource (Dutta et al., 2017). Besides, the roll-out of CO<sub>2</sub> utilization is highly dependent on the decreased cost of hydrogen production in the future, and the literature features some very diverging assumptions regarding future trends (IRENA, 2020; Schmidt et al., 2017). It is up to modelers to make more or less strong assumptions on the evolution of costs for both low-carbon electricity and hydrogen over time. The decrease in costs can be justified by assuming the future scaling of processes as well as research funding for more efficient CO<sub>2</sub> utilization processes (Cuéllar-Franca et al., 2019). As for many novel technologies, process scaling is a well-known lever to improve the efficiency of processes and reduce costs (Kim, 2021; Mauler et al., 2021; Yoshida et al., 2021). This strategy is also recommended for CCU (Cuéllar-Franca et al., 2019; Luna et al., 2019). We argue that such assumptions should be formulated and justified in the context of specific modeling scenarios in which either high or low performances for hydrogen and electricity are assumed. Secondly, we point out the importance of building so-called "CO<sub>2</sub> hubs", which consist in concentrating the industries requiring CO<sub>2</sub> as feedstock with other CO<sub>2</sub>-emitting industries equipped with CO<sub>2</sub> capture units within a nested web. The concept involves creating synergies between capture units, renewable energy generation and smart grids (Sandalow et al., 2019), in order to improve the overall efficiency and reduce the costs of the infrastructure web, notably for CO<sub>2</sub> transportation (Bui et al., 2018; IEA, 2019c). This consideration could steer CCU in energy models and will in any case need to be modeled, as such hubs are currently in development in Europe (IOGP, 2019).

Over and above technical levers, the development of CCU in energy models could also benefit from policies. As a matter of fact, Table 1 shows that energy models provide poor information about climate policies in favor of developing CO<sub>2</sub> utilization. Indeed, except for some models that consider a carbon tax (Leonzio et al., 2019; Quarton and Samsatli, 2020), or others studying the impact on CO<sub>2</sub> storage unavailability (Blanco et al., 2018a; IEA, 2019b), the modeling of CO<sub>2</sub> utilization is not addressed within a specific climate policy, unlike incentives for renewable technologies or a planned deployment rate. (Keppo et al., 2021) acknowledge that policies other than carbon pricing are usually not present in all IAMs, especially local or sector-specific ones, hence biasing the outcome of the models. The following list enumerates three main policy levers that would drive CO<sub>2</sub> utilization deployment in the results of energy models.

1. **CO<sub>2</sub> pricing or carbon taxation**

A major policy lever is the implementation of a carbon tax that would attribute a value to CO<sub>2</sub> emissions of \$40-\$80/tCO<sub>2</sub>. Henceforth, a major issue arises: how do we measure CO<sub>2</sub> emissions reduction when the sequestration of CO<sub>2</sub> in a product is not permanent, and how do we account for negative emissions? Because each CCU route may have different environmental benefits, we argue that a CO<sub>2</sub> price should be indexed for each CO<sub>2</sub>-based product depending on its climate benefit, indicating once more the need for robust LCAs. This issue still needs to be addressed by modelers.

2. **Policy incentives**

Policy incentives can take various forms, such as tax credits, product labelling, R&D funding or direct government funding for projects (ICEF, 2016). In this area, we observe that it is very simple in energy modeling to incentivize the production of CO<sub>2</sub>-based goods with subsidies by lowering the investment cost (CapEx) in CCU assets, or by lowering the production cost to a certain level. It remains for modelers to decide on the magnitude of these incentives, for example by working with sensitivity analyses. However, researchers warn not to incentivize CCU projects unless a robust life-cycle assessment of emissions savings has been performed upstream (Hepburn et al., 2019; IEA, 2020).

3. **Legal and policy framework**

Finally, a policy framework, as well as a legal framework, should be built globally (Nakamura et al., 2019) to ensure fair competitiveness between actors, and to avoid regional actors being penalized by others. Although necessary for the successful development of CCU, this lever seems hard to model. However, one might imagine for a given scenario that all agents from all regions in all sectors of the energy system modeled are constrained by the same climate policies. For IAMs modeling both the climate and the world energy system, a simple way to consider a legal framework is to constrain the energy system to its related GHG emissions so that the temperature of the globe does not exceed a certain level. Similarly, one can imagine that all sectors are bound to a net-zero target. Consequently, all agents are forced to transition fairly and CCU has more chance of being revealed as a significant contributor to this goal.

Thus, modelers can draw on the technical and political parameters that emerge in real projects and incorporate them into the modeling. However, we call on modelers to be transparent about assumptions in relation to the overall CCU chain.

### **4.3. Recommendations for CCU modeling**

For new modelers seeking to represent CCU in energy models as a novel alternative, we make the following recommendations.

At the first link of the CCU chain, CO<sub>2</sub> capture must be represented as broadly as possible in order to identify the source of CO<sub>2</sub> (either fossil, process-related, atmospheric, native or biogenic) and quantify

the CO<sub>2</sub> capture requirements. The latter is essential to fully estimate the total CO<sub>2</sub> to be captured and the former is also important to identify the strategic CO<sub>2</sub> point sources to capture before using it. In other words, the capture of CO<sub>2</sub> must be modeled at every possible level of the energy system considered. In a broader sense, CCU needs to be modeled in global models to assess the full potential. Of the 22 models reviewed in the present study, we note 9 global models including CCU technologies worldwide. Given the large number of global models (more than 29) in the research community (UNFCCC, 2021), we can deduce that CO<sub>2</sub> utilization is poorly represented at the global level. Table 1 shows that Europe is the geographical area of greatest interest for the utilization of CO<sub>2</sub>. Moreover, as mentioned in Section 1, if CCU is considered in any model or study, it is implemented as an option to decarbonize a particular sector of the economy, e.g. the chemical sector or transport, but not for all sectors. Therefore, it is currently hard to assess the complete potential of CCU across all continents and all sectors, which can be detrimental for estimating the requirements of capture units, whereas CCU is modeled to this purpose (Section 1). We thus strongly recommend the complete integration of CCU, i.e. including all types of CO<sub>2</sub>, for all sectors and all regions of the world. Bottom-up models and specifically global TIMES models are suited for such a task because they deal with energy and material flows (Loulou and Labriet, 2008). The origin of CO<sub>2</sub> can be identified and tracked so that modelers can easily analyze from the results the role of CCU depending on the origin of the CO<sub>2</sub>.

As the second link of the CCU chain, we note a clear interest in CO<sub>2</sub> utilization for the transport sector and the manufacture of fuels, with regard to the overview of current models. Indeed, shifting to clean fuels and enhancing energy efficiency are crucial measures to reduce emissions from this sector and avoid having to replace the entire fleet (van Vliet et al., 2011). The power sector could also abate its CO<sub>2</sub> emissions with renewable energies or nuclear power. However, the industry sector has no choice but to rely on CO<sub>2</sub> capture at some point, because of the difficulty of abating its process emissions. It remains to be decided whether it is more interesting to store or to utilize the captured CO<sub>2</sub>. Heavy industries could benefit from CCU to produce clean chemicals, reduce carbon footprints of cement and concrete, and enhance steel slags to increase their sales. As industry is one of the most difficult sector to decarbonize, CCU offers a milestone to define a mitigation strategy, considering all the possible routes. We thus call upon modelers to make efforts to represent CO<sub>2</sub> utilization as broadly as possible for the industrial sector. The challenge is even greater given that most CO<sub>2</sub> utilization processes are exothermic (specifically in the hydrogenation of CO<sub>2</sub> to produce fuels), meaning that the residual heat can be reused within the process of the asset or directly utilized at the capture or electrolysis unit. This strategy could be a game changer for CCU modeling. Beyond the integration of heat, an overall, gate-to-gate CCU process would benefit from several different integrations that still need to be optimized and assessed to determine the most profitable design (Cuéllar-Franca et al., 2019). The integration of CO<sub>2</sub> utilization processes is thus crucial to model, in order to get the most out of it. In addition to modeling the implementation of brand-new, stand-alone CCU facilities, we strongly recommend modeling the retrofitting of current industrial assets which have long lifespans. Instead of abandoning existing assets with a high economic impact, retrofitting existing assets might be an opportunity for CCU technologies and should be considered. In the meantime, energy models usually only incorporate the investment in new capacities as a major decision variable, while the retrofitting of existing assets is barely considered. Therefore, we argue that modelers should also consider the retrofitting of current long-life assets, and not only investment in expensive new capacities for the industry.

Apart from the technical modeling recommendations, we argue that CCU could be modeled in other contexts, such as the sustainability of the economy or a carbon circular economy. Firstly, TEAs and LCAs currently make up much of the research about CCU performance (Cruz et al., 2021), while the socio-economics of CCU raises less interest (Centi et al., 2020). This could be one reason why TD models are underrepresented in CCU modeling: they need this kind of information in order to be run. TD models have the potential to enrich the debate with further insights on the impacts of CCU roll-out on GDP, employment, fuel prices or consumption, all of which would help to assess whether CCU is

an interesting technology to be deployed for socio-economic and environmental concerns. Currently, the results of BU models are oriented through a prism of techno-economic feasibility and the potential environmental benefits of CCU, and are likely to be challenged by the results of TD models. Secondly, we notice that CO<sub>2</sub> utilization has never been studied in energy models in the context of a carbon circular economy, as George Olah proposed (Olah et al., 2009). The concept is to develop an economy based on the utilization of carbon coming solely from atmospheric CO<sub>2</sub> rather than fossil fuels to satisfy our needs for fuels and other products by converting the captured carbon with clean energies. In this paradigm, the extraction and use of fossil fuels would not be needed anymore, as the world would only rely on atmospheric CO<sub>2</sub>. Gulf countries are particularly interested in the carbon circular economy due to their high potential for solar and renewable energies, making it easier to both capture CO<sub>2</sub> and convert it with clean energies (Al-Alawi et al., 2020; Al-Sadoun, 2019; Al-Saidi et al., 2021). However, we have not identified any study that has run an energy model including CCU in the Middle East region (Table 1). If CCU were modeled in the context of a carbon circular economy, the potential for capture and use of CO<sub>2</sub> is likely to be much larger than it would be in the context of emissions reduction; we argue that the potential of CCU assessed in either context should be confronted and discussed. Thirdly, as mentioned in section 4.2, the modeling of CO<sub>2</sub> hubs would be interesting for VCMs. Indeed, the entire set of VCMs we reviewed considers sparse capture sites and storage sites that require expensive CO<sub>2</sub> pipelines to link them to each other, while the cost could be minimized with CO<sub>2</sub> hubs. We believe that the results that VCMs obtain should be compared with cases where capture, utilization, and storage sites are concentrated into hubs.

As for policy concerns, we discussed before that a legal framework is essential to promote CCU. A first step was achieved when most countries in the world ratified the Paris Agreement in 2016. All countries must now set national targets corresponding to their engagement, and ensure social acceptability and public awareness. However, in reality, some regions of the world will transition more rapidly and earlier than others. In the case of CCU, North America, Western Europe and Eastern Asia are already showing an interest in CO<sub>2</sub> utilization. Therefore, especially for global models, we argue that both incentives and climate policies should be addressed to these regions of the world as a priority. This would render the results more realistic.

**Note that the review we performed is based on the analysis of 22 studies.** We are aware that our inferences are based on a non-exhaustive overview of the literature, which may bias our argument.

## 5. Conclusion

In response to climate urgency and the formulation of more stringent climate constraints embodied by the Paris Agreement, decision makers must inevitably find new levers and develop new strategies. Carbon capture and utilization technologies are of interest for both mitigating emissions and generating revenues. In order to develop this technology, an assessment of CCU potentials and performances needs to be researched, not only through TEA and LCA studies, but also employing energy models because of their ability to integrate several facets of an overall energy system.

However, our review shows that the complete representation of CCU is absent from energy models. In particular, top-down models need to make an effort to better understand the socio-economic effects of its potential deployment. Also, in order to better quantify CO<sub>2</sub> capture capacities, we argue that CCU needs to be modeled at all possible capture sites and for all CO<sub>2</sub> utilization processes. Although indispensable, the modeling of CO<sub>2</sub> capture does not systematically include biogenic and atmospheric CO<sub>2</sub>, and the modeling of CO<sub>2</sub> utilization mainly addresses the production of fuels and chemicals while leaving aside other key utilizations for industry. Moreover, CCU should be further explored at the global level.

Consequently, decision-making in favor of CCU seems to be hazardous at this point in time. As CO<sub>2</sub> utilization has been demonstrated to be an immature technology currently more suited to the medium

term, we believe that the research modeling community still has time to study the matter of CCU in all of its complexity before advising decision-makers to gamble on CCU with major investment plans.

Such models can only be developed if the scientific community focuses on the economic and environmental quantification of the performance of CO<sub>2</sub> utilization processes. We therefore call for deeper research to produce LCA and TEA studies on the range of options available for CO<sub>2</sub> utilization. Finally, this paper provides references for CCU modelers in search of data and recommends good practices and further helpful developments in CCU modeling.

### **CRedit author statement**

**Lucas Desport:** Conceptualization, Methodology, Investigation, Visualization, Writing - Original Draft, Writing - Review & Editing. **Sandrine Seloisse:** Conceptualization, Supervision, Writing – Review & Editing.

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