



Decarbonization in Complex Energy Systems: A Study on the Feasibility of Carbon Neutrality for Switzerland in 2050

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Decarbonization gained prominence with the witnessed rise of temperature over recent years, particularly in the aftermath of the adoption of the Paris agreement for limiting the temperature increase within 2°C until 2050. Biogenic resources are explicitly indicated as carbon-neutral from Life Cycle Assessment perspective by the IPCC, shedding light on the carbon-neutral society by applying Biogenic Energy Carbon Capture for creating negative emissions. This article proposes a novel modeling approach by introducing carbon layers with specification on the principal carbon sources and sinks based upon an optimization algorithm, in order to solve the carbon loop issue in a highly interconnected energy system due to increasing penetration of biomass and carbon capture, use, and storage. This study contributes to quantifying biogenic and nonbiogenic carbon footprints, and optimizing the circular economy associated with a net-zero-emission society, in favor of policy-making for sustainable development in long terms.

Keywords: carbon neutrality, carbon capture, use, and storage, circular carbon flow, energy planning, biogenic energy with carbon capture, mixed-integer linear programming optimization

1. INTRODUCTION

Carbon mitigation is becoming an essential and urgent issue in human activities, infiltrating into various societal fields, including politics, culture, economy, environment, lifestyle, ecology, resource, and so on. In the context of striving for a sustainable society, participating countries in the Paris Climate Summit which took place in 2015 reached an agreement, declaring the objective of keeping the increase in global average temperature to well below 2°C above preindustrial levels within this century, and further to pursue efforts to limit the increase to 1.5°C (IPCC, 2014). In this context, European countries are pioneering the exploration of plausible pathways toward carbon mitigation: the Netherlands announced that all Dutch cars must be emission free by 2030 (NLTimes, 2017); Germany planned to phase out the coal power plants by 2038 (Rinscheid and Wüstenhagen, 2019); and the Danish government decided to provide 100% of Denmark's energy requirements in electricity, heating, and transport from renewable sources by 2050 (Madsen et al., 2018). In terms of Switzerland, there is a host of energy policies that range from rules for market liberalization to programs for energy conservation, subsidies for renewables, and regulations for CO₂ reduction (Markard et al., 2016). In 2011, the Swiss government and parliament decided to phase out nuclear power plants following the Fukushima nuclear accident, and to stimulate energy

efficiency and the use of renewable energies instead. As a consequence, the government developed the Energy Strategy 2050, setting long-term targets for the reduction of energy consumption (54% reduction until 2050) and the expansion of renewable electricity generation and combined generation of power and heat. Concerning climate policy, Switzerland undertook a commitment to halve its greenhouse gas emissions vs. the 1990 level by 2030. To accomplish this, the existing Federal CO₂ Act has to be revised for the period beyond 2020. The corresponding bill is currently being debated in Parliament. In 2019, the Swiss Federal Council resolved that, as of 2050, Switzerland is to reduce its net greenhouse gas emissions to zero (net-zero-emission target) (SFOE, 2020). This declares it is aiming to meet the internationally agreed goal of limiting global climate warming to a maximum of 1.5°C vs. the preindustrial period. To realize this objective, two methods are generally considered:

- mitigation of carbon sources: predominately translated by the massive penetration of renewable resources, and efficiency improvement for carbon-intensive areas;
- reinforcement of carbon sinks: in either natural way, such as afforestation and reforestation, or artificial way, typically the deployment of CCUS technologies.

Therefore, it is necessary to analyze the carbon flows of the energy system, by distinguishing carbon categories and identifying various carbon sources and sinks. This article proposes a modeling approach by defining specific carbon layers based upon distinguished carbon categories and identified carbon sources and sinks, in order to clarify the murkiness in energy system models on carbon loop issues, especially in the context of increasing biogenic energy with carbon capture (BECC) where the biomass serves as both a carbon source and a sink. This approach contributes to quantifying the carbon footprints of the system and discovering potential opportunities for a breakthrough, especially with respect to certain key technologies.

This article hereafter is organized in the following way: **Section 2** resumes the state-of-the-art from the literature review; **Section 3** clarifies the modeling methodology for the MILP (mixed-integer linear programming) optimization, with specification on the carbon flow modeling; **Section 4** presents the key data and assumptions used in this research; **Section 5** defines decarbonization scenarios and analyzes the results, followed by a discussion on how to achieve carbon neutrality; at last, a conclusion is drawn in **Section 6** by resuming the core achievements and limitations of the research.

2. STATE-OF-THE-ART

With increasing attention to the decarbonization of the energy system, numerous articles mentioned the essence of biomass playing in achieving this goal. National Academies of Sciences, Engineering and Medicine (2018) emphasized two technologies for converting biomass to fuels, namely, pyrolysis and

gasification; other possible technologies, such as biomass Fischer–Tropsch processes, hydrothermal gasification, etc., had yet not been accounted for. Celebi et al. (2017) reviewed and analyzed various lignocellulosic biorefineries and suggested process design methodology for improving thermo-environmental performance, which is nevertheless not able to quantify the impact of these improvements on the multisector energy system structure. Dahiya et al. (2018) proposed a concept of circular bio-economy with biorefinery, which focused merely on the biomass field, without analysis on the impact of the biomass on the whole energy system. Similar topics include Pfeffer et al. (2007), Santibañez-Aguilar et al. (2011), and Peduzzi (2015). Smith (2016) came up with seven scenarios elaborating fossil CCS (carbon capture and storage) and BECCS, and the production of biofuels, but no further information on how to optimize the usage of the synthesized biofuels, and their corresponding impact to the other energy conversion technologies. In parallel, Creutzig et al. (2015) emphasized the role that CCS plays in biogenic carbon treatment, but ignored the possibility of CCU application. Instead, SAPEA (2018) took into account the role of CCU, but simply concluding the CCU is not able to abate the carbon emission, since the captured carbon is finally released back to the atmosphere, where the effect of the decreased utilization of fossil fuels is neglected.

Concerning BECC, the majority of current researches focus principally on the improvement of the performance of standalone BECC processes within limited boundaries, for instance at an industrial site level, rendering a lack of holistic view on the interactive impacts on the whole energy systems. Another challenge is arising with the increasing advocacy for carbon capture and utilization (CCU), which unavoidably releases back the captured carbon into the atmosphere, resulting in carbon flow loops as long as the carbon products are not chemically stable and nonreleasable, typically recyclable plastics. The loop issue is even more tough to be tackled taking into consideration the double nature of biomass as both carbon source and sink. In addition, current studies have paid limited attention to the relationship of carbon capture and renewable development, which cannot be simply regarded as *synergistic* or *mutually exclusive* due to the intrinsic complexity of the interactions between resources and technologies.

As to the modeling of carbon flows, the majority of articles are dedicated to depicting the inter-regional import and export of carbon fuels, such as Aichele and Felbermayr (2010), Ackerman et al. (2007), and Chen et al. (2017), with limited attention on the intrinsic complexity of the energy system. Some focused on carbon economics on the market such as Spaargaren and Mol (2013) with up-bottom approaches, rendering a lack of details on the technological aspects of the system. Gounand et al. (2018) analyzed the impact of carbon flows on the ecosystems, with limited information on the energy sides; Chen and Chen (2017) emphasized the correlation between energy consumption and carbon emissions; however, the proposed methodology is still an acyclic model, implying circular carbon flows are not considered. Ramaswami et al. (2011) and Suciú et al. (2018) analyzed the carbon footprints within city scale, which is yet difficult to be

generalized into a national level, which requires scrutiny since limited freedom of technologies and resources in small cases may restrict the flexibility of a system with diverse possibilities.

Currently, many researchers demonstrate that decarbonizing a specific energy sector within limited boundary is feasible, such as Schiffer and Manthiram (2017) for chemical industry, Braune et al. (2019) for building, and Hannula and Reiner (2017) for transport. However, it should be highlighted that decarbonization of a certain sector may not be substantially beneficial to the decarbonization of the whole energy system, since it might simply shift the carbon emission from one sector to other sectors. For instance, a steel-manufacturing factory opts to consume more electricity than conventional coal/gas as energy carriers in order to mitigate carbon emission, which in nature is risky of transferring the emission pressure to the power sector if the electricity mix is still fossil-dominant. Up to now, there are few models capable of studying circular carbon flow in complex energy systems with multisectors for quantifying the impact of increasing penetration of biogenic carbon sources with CCUS.

From the authors' perspective, a holistic model allows for an in-depth exploration on the interaction between approaches, some of which are supposed to be mutually exclusive; e.g., the implementation of CCS is likely to be impeded by the increasing penetration of intermittent renewables due to lack of available carbon sources, while some are reckoned synergistic, e.g., the development of storage technologies is expected to be in parallel to the renewables' evolution. Therefore, without a holistic view of the whole system, it is difficult to judge the role of a standalone process/sector in the energy transition.

Conventional methods for dealing with complex systems involve simulation and optimization: Simulation is the most straight-forward method with computational efficiency competence for projection modeling by fixing assumptions and observing the consequent pathways. Its application is however limited particularly in the presence of loop problems, where it is difficult to get the optimal solution from limited tests; conversely, optimization deals with a problem by exploring part of (or the whole) feasible zone at a sacrifice of heavy computational complexity and is commonly used as an auxiliary tool for decision-making. Additionally, an optimization problem can be transformed into a simulation problem by enforcing constraints. Taking into consideration the multilateral interactions in the energy systems, an optimization model based upon AMPL (A Mathematical Programming Language) was applied in this research and is elaborated in Section 3.

3. MODELING METHODOLOGY

3.1. Model Description

3.1.1. General Introduction

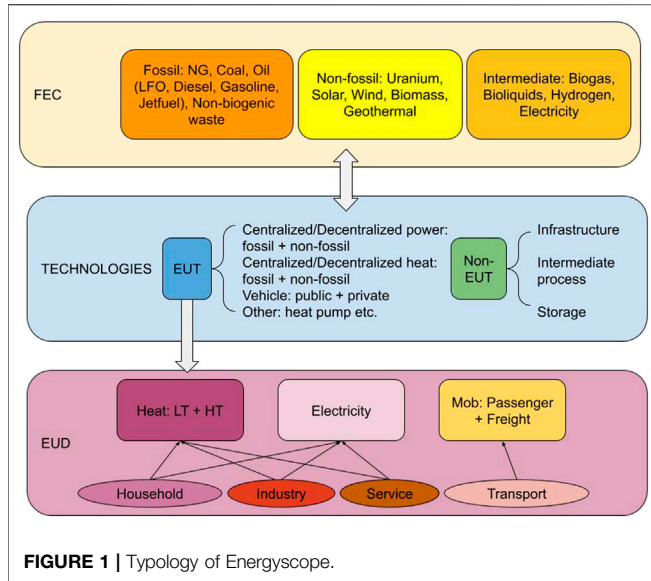
This research is conducted based upon Energyscope, a bottom-up energy system model developed in the Industrial Process and Energy Systems Engineering (IPESE) group in favor of decision-making for techno-economic and ecological

optimization. Compared to other existing energy models, which are often proprietary, computationally expensive, and mostly focused on the electricity sector (Limpens et al., 2019), Energyscope optimizes both the investment and operation strategies of an entire energy system (including electricity, heating, and mobility) by taking a "snapshot" for a given objective year. In this study, the time horizon in consideration is 2050 with a monthly resolution. Having a good performance in the trade-off between the modeling scope and computational time, Energyscope was applied to analyze the uncertainty by Moret et al. (2017) and Li et al. (2019). This open-source platform provides users with the flexibility to define tailored scenarios and analyze the corresponding economic and ecological impacts.

In this model, we highlight the difference in final energy consumption (FEC) and end-use demand (EUD). FEC is defined as the amount of input fuel needed to satisfy the EUD. For instance, FEC refers to, in an oil heat boiler, the amount of oil consumed, while EUD corresponds to the heat generated. The efficiency of the boiler is thus defined by the ratio of EUD over FEC. As presented in **Figure 1**, the EUD in Energyscope covers the process heat (HT), low-temperature heat (LT), including space heating and hot water supply, electricity, passenger mobility, and freight mobility, where space heating varies in different months according to the distribution ratios given by Moret et al. (2017), while the other demands are supposed to be uniformly distributed within the whole year. In Energyscope, the links between FEC and EUD are bridged by end-use technologies (EUT), such as the boiler aforementioned. One technology can have multi-inputs and outputs, e.g., a cogeneration gas plant provides both heat and electricity with corresponding efficiencies. Additional to EUT, a part of technologies are responsible for intermediate conversions without direct participation in supply for EUD, such as the storage technologies. From the FEC side, Energyscope involves 1) fossil fuels: natural gas, coal, nonbiogenic waste, heating oil, diesel, and gasoline; and 2) nonfossil resources: uranium, solar, wind, geothermal, and biomass. Intermediate resources include electricity, hydrogen, biogas, and bio-liquids (gasoline and diesel). In particular, electricity is regarded as a resource if it serves as an input of one technology, for instance in the electrolysis process; or as an EUD by household appliances. Specifically, CO₂ is of double nature in this model: It is regarded as an output associated with positive-emission technologies, and as an input resource in negative emission technologies such as synthesizing fuels/plastics. In order to simulate the energy/mass flows, the concept of layers is introduced, which serves as dynamic tanks for balancing all the inputs and outputs in each time period taking into account corresponding conversional efficiencies. Detailed mathematical interpretation of the layers' behavior is presented in **Section 3.1.2**.

3.1.2. Mathematical Formulation

In this article, all decision variables are marked in bold format. The objective function of the Energyscope is to minimize the



annual total cost C_{tot} expressed by the sum of the annualized CAPEX (C_{inv}), the annual fixed OPEX for the maintenance (C_{maint}) and the annual variable OPEX costs (C_{op}) for purchase of resources, as shown in Eq. 1, where the sets \mathcal{E} , \mathcal{R} , and \mathcal{T} represent the technologies, the resources (renewables and non-renewables as well as electricity import) and the time periods (twelve months within one year), respectively. $t_{op}(t)$ denotes the duration of the period t . The investment cost $C_{\text{inv}}(j)$ is annualized by a factor $\tau(i, n(j))$ expressed in Eq. 2, with i the discount rate assumed to be 2.215% and $n(j)$ the expected lifetime for the technology j . The investment cost and fixed operational cost (maintenance) for a given technology are proportional to its installed capacity $F(j)$, which defines the annual capacity factor $cp(j)$ in Eq. 3 as the ratio of the annual production (by summing the power output $F_t(j)$ in GW multiplied by the corresponding period duration $t_{op}(t)$, $t \in \mathcal{T}$) over the theoretical annual production at full load. The annual output $F_a(j)$ is expressed as the sum of monthly outputs. As to the variable operational cost, it depends on the amount of resources consumed, and specific cost for each resource (nonrenewable and renewable) available in the **Supplementary Material**. It should be highlighted that the monthly outputs of intermittent renewable technologies ($j \in \mathcal{I}$), namely, solar and wind as well as hydro power, are limited by the corresponding monthly capacity factor $cp_t(j)$. Other constraints include: the proportional relationship of investment cost and the installed capacity by Eq. 6 for every technology in consideration; the same for maintenance cost (fixed OPEX) by Eq. 7. Each technology emits GHG during their construction period, which is noted by $\text{GWP}_{\text{constr}}$ and is also assumed to be in line with its installed capacity by Eq. 8, which is scaled by Eq. 9 between its minimal and maximal values. Different from the investment and maintenance cost, the variable operational cost is decided by the sum of purchase amounts of resources in each period as expressed in Eq. 10, and

the availability of resources is capped by Eq. 11. For example, the availability of waste for incineration is limited to an upper bound determined by the population. Equation 12 reflects the concept of layer balance in each period, where $f(i, l)$ stands for the conversional efficiency of a technology i contributing to a certain layer $l \in \mathcal{L}$, or for the resource purchase if $i \in \mathcal{R}$ and $i = l$ where f is set to be 1. Take electricity layer as an example, the layer's level at time period t is expressed as the sum of import (positive value for f), the domestic production by technologies (positive value for f , such as by PV) and internal consumption (negative value for f , such as by an electric heat pump), which is supposed to match the EUD for electricity in the same period. DHN installed capacity is decided by two aspects: 1) it is defined as a value larger than or equal to the total installed capacity of all DHN technologies by Eq. 13; 2) taking into account the energy supply security, DHN should be more than "just enough" in order to meet the demand in peak period, and as a result, a peak parameter $\%_{\text{peak}}$ is defined in Eq. 14, and in this model, we assume it to be 200% of the maximal district heating demand. Energy loss is considered in Eq. 15, where \mathcal{G} stands for the electricity and district heating. It is assumed the electricity loss in each period is proportional to the total production from all the power generation technologies, the same for DHN heat loss. In terms of Switzerland, we assume the loss percentages ($\%_{\text{loss}}$) 7% and 5% for electricity grid and DHN network, respectively.

$$\min C_{\text{tot}} = \min \left(\tau(i, n(j)) \sum_{j \in \mathcal{E}} C_{\text{inv}}(j) + \sum_{j \in \mathcal{E}} C_{\text{maint}}(j) + \sum_{r \in \mathcal{R}} \sum_{t \in \mathcal{T}} C_{\text{op}}(r, t) \right), \quad (1)$$

$$\tau(i, n(j)) = \frac{i(1+i)^n(j)}{(1+i)^n(j) - 1}, \quad (2)$$

$$F(j)cp(j) \sum_{t \in \mathcal{T}} t_{op}(t) \geq \sum_{t \in \mathcal{T}} (F_t(j)t_{op}(t)) \quad \forall j \in \mathcal{E}, \quad (3)$$

$$F(j)cp_t(j) \geq F_t(j) \geq 0 \quad \forall j \in \mathcal{I}, t \in \mathcal{T}, \quad (4)$$

$$\sum_{t \in \mathcal{T}} F_t(j)t_{op}(t) = F_a(j) \quad \forall j \in \mathcal{E}, \quad (5)$$

$$C_{\text{inv}}(j) = c_{\text{inv}}(j)F(j) \quad \forall j \in \mathcal{E}, \quad (6)$$

$$C_{\text{maint}}(j) = c_{\text{maint}}(j)F(j) \quad \forall j \in \mathcal{E}, \quad (7)$$

$$\text{GWP}_{\text{constr}}(j) = \text{gwp}_{\text{constr}}(j)F(j) \quad \forall j \in \mathcal{E}, \quad (8)$$

$$f_{\text{min}}(j) \leq F(j) \leq f_{\text{max}}(j) \quad \forall j \in \mathcal{E}, \quad (9)$$

$$C_{\text{op}}(i) = \sum_{t \in \mathcal{T}} c_{op}(i, t)F_t(i)t_{op}(t) \quad \forall i \in \mathcal{R}, \quad (10)$$

$$\sum_{t \in \mathcal{T}} F_t(i)t_{op}(t) \leq \text{avail}(i) \quad \forall i \in \mathcal{R}, \quad (11)$$

$$\sum_{i \in \mathcal{R} \cup \mathcal{E}} f(i, l)F_t(i) - \text{EndUses}(l, t) = 0 \quad \forall l \in \mathcal{L}, \forall t \in \mathcal{T}, \quad (12)$$

$$F(\text{DHN}) \geq \sum_{j \in \text{DHN_TECH}} F(j), \quad (13)$$

$$F(\text{DHN}) \geq \%_{\text{peak}} \max_{t \in \mathcal{T}} \{\text{EndUses}(\text{HeatLowTDHN}, t)\}, \quad (14)$$

$$\text{Loss}(\mathbf{g}, t) = \left(\sum_{i \in \mathcal{R} \cup \mathcal{E} | f(i, \mathbf{g}) > 0} f(i, \mathbf{g}) \mathbf{F}_t(i) \right) \%_{\text{loss}}(\mathbf{g}) \quad (15)$$

$$\forall \mathbf{g} \in \mathcal{G}, \forall t \in \mathcal{T},$$

$$\mathbf{F}_t(j) + \mathbf{F}_t(k) \mathbf{Y}_{\text{Solar}}(j) \geq$$

$$\frac{\text{EndUses}(\text{HeatLowTDHN}, t) + \text{EndUses}(\text{HeatLowTDec}, t)}{\text{endUsesInput}(\text{HeatLowTSH}) + \text{endUsesInput}(\text{HeatLowTHW})}$$

$$\sum_{t \in \mathcal{T}} \mathbf{F}_t(j) t_{\text{op}}(t),$$

$$k = \text{DEC}_{\text{Solar}}, \forall j \in \text{HeatLowTDec}, j \neq k, \forall t \in \mathcal{T} \quad (16)$$

$$\sum_{j \in \mathcal{E}} \mathbf{Y}_{\text{Solar}}(j) \leq 1, \quad (17)$$

$$\mathbf{F}(\text{GRID}) = 1 + \frac{9400}{c_{\text{inv}}(\text{GRID})} \frac{\mathbf{F}(\text{WIND}) + \mathbf{F}(\text{PV})}{f_{\text{max}}(\text{WIND}) + f_{\text{max}}(\text{PV})}, \quad (18)$$

$$\begin{aligned} \text{STO}_{\text{in},r}(t) + \text{STO}_{\text{out},r}(t) &\leq 1 \quad \forall t \in \mathcal{T} \\ 0 \leq \mathbf{F}_{t,\text{in}}(j) &\leq \text{STO}_{\text{in},r}(j, t) \mathbf{F}(j) \eta(j) \quad \forall j \in \mathcal{S}_r, \forall t \in \mathcal{T}, \\ 0 \leq \mathbf{F}_{t,\text{out}}(j) &\leq \text{STO}_{\text{out},r}(j, t) \mathbf{F}(j) \eta(j) \quad \forall j \in \mathcal{S}_r, \forall t \in \mathcal{T} \end{aligned} \quad (19)$$

$$\begin{aligned} \mathbf{SL}_r(t) &= \mathbf{SL}_r(t-1) + \mathbf{F}_{t,\text{in}}(j) t_{\text{op}}(t) - \mathbf{F}_{t,\text{out}}(j) t_{\text{op}}(t) \\ &\forall j \in \mathcal{S}_r, t \in \mathcal{T}. \end{aligned} \quad (20)$$

A couple of constraints are dedicated for renewable energies. **Equations 16** and **17**, expressed in a compact nonlinear formulation, where the nominator and denominator represent the low-temperature heat demand in month t and in the whole year, respectively, render the model more realistic by defining the operating strategy for decentralized heating: the relative use of each technology in each period should be constant, except for the solar thermal (DecSolar): if solar thermal k is installed ($\mathbf{Y}_{\text{Solar}} = 1$), then at maximum, one technology j is used as backup. In order to reflect the impact of increasing penetration of intermittent renewables, particularly PV and wind, we assume the scale of power grid as a linear function expressed by **Eq. 18** in correspondence to the total installed capacity of PV and wind, with a specific additional investment cost of 9.4 billion CHF according to Moret (2017). Additionally, with increasing penetration of renewables, seasonal storage is regarded as an effective method in transferring excessive energy from peak to deficit periods. The technologies for seasonal storage in Energyscope involve: hydrogen storage and natural gas storage. Short-term storage, such as pumped hydro and battery storage, is not considered in the model due to time resolution incompatibility, typically in hourly or daily granularity. The lack of short-term storage technologies are not supposed to have obvious influence on the monthly-modelling results: on one hand, it is difficult to precisely predict the daily or hourly behaviors of the energy system in 2050, while the monthly-level data contribute to the alleviation of short-term fluctuations and by consequence regarded more stable; on the other hand, the short-term storage serves only as buffer and occurs merely in the daily level, implying no influence on the monthly net energy surplus or deficit that is determined by the difference of monthly demand and production. The associated data for the long-term storage technologies are listed in **Table 1**. In order to model the

TABLE 1 | Storage cost, summarized from Gorre et al. (2018) and Leeuwen and Zauner (2018).

	Storage method	c_{inv}^a (€/kWh)	$c_{\text{op, maint}}$ (€/kWh)
Hydrogen	Salt caverns	0.036	0.00072
	High-pressure steel tanks ^a	33.33	0.49995
Methane	Depleted natural gas reservoir	0.009	0.00018
	Salt caverns	0.012	0.00024
	High-pressure steel tanks ^b	10.78	0.2156

^aThe investment cost is based upon the maximal volume of storage, multiplied by the specific investment cost.

^bBased upon 100 €/m³ capital expenditures; not integrated into Energyscope since it is commonly used for short-term storage.

dynamics of the storage behavior of the energy system, two binary variables $\text{STO}_{\text{in},r}$, $\text{STO}_{\text{out},r}$ were introduced for the three storage resources r , respectively, subject to the constraints defined in **Eq. 19**. STO_{in} is set to be one in a storage-dominant month, and in correspondence STO_{out} is assigned to be zero in the same period. As a result, $\mathbf{F}_{t,\text{in}}$ represents the net storage (storage-release). Vice versa for a release-dominant month. This approach rules out the possible simultaneous storage and release within each period due to independent operations in different plants, facilitating the modeling on a national scale. Here, \mathcal{S}_r represents the storage technologies (storing and releasing) for the resource r , and η denotes the capacity factor. Since the last two constraints in **Eq. 19** are *quadratic*, rendering the problem into an MINLP (Mix Integer Non-linear Programming), eight equivalent equations are introduced for linearizing the quadratic model in order to achieve computational effectiveness without loss of quality. The accumulated storage level SL for each storage resource r is given by a time-continuous and cyclic **Eq. 20**. Other constraints dedicated to carbon flows will be explained in **Section 3.2**.

3.2. Carbon Flow Modeling

This section focuses on presenting the modeling approach for circular carbon flows in energy systems. The major carbon sources and sinks, as well as key technologies, are analyzed in **Sections 3.2.1.–3.2.4**, followed by **3.2.5** presenting the modeling concepts of carbon layers in Energyscope. In order to quantify the carbon flows, a parameter named carbon content linking the energy and carbon mass for each carbon resource and product r is defined by **Eq. 21**:

$$\text{carbon content}_r = \frac{m(C)}{m(r) \cdot \text{LHV}_r} \quad (21)$$

where the $\frac{m(C)}{m(r)}$ denotes the carbon element mass fraction (%) of r , and the LHV_r refers to its *lower heating value*. Without specification, all mass-energy conversion in this article is based upon LHV .

Carbon management is considered by taking into account various carbon-containing resources, either biogenic or nonbiogenic, carbon sinks in the form of CO₂ capture technologies, CO₂ emissions from biomass conversion, as well as CO₂ utilization to produce synthetic chemicals and fuels. Apart from the conventional carbon balance between sources and sinks,

conversion of biogenic resources yields useful energy products but also CO₂ that can be considered a waste stream, which can be further transformed into useful products via different chemical synthesis routes. Both these conversion technology groups are used in the Energyscope model to fulfill a two-fold purpose. On one hand, the produced fuels and products from biomass or CO₂ are used to substitute fossil carbon with biogenic one, thus reducing the needs for conventional fossil resources, while at the same time, the circular utilization of CO₂ within the energy system itself leads to a significant reduction of the overall carbon emissions to the atmosphere. The use of Eq. 21 enables not only the quantification of the carbon in each of the system flows, but also provides a method to help track the footprint of these contributing flows within the complex energy system.

3.2.1. Carbon Sources

- Biogenic carbon sources, including
 - (1) domestic wood: waste wood, wood residues, and forest wood (soft and hard);
 - (2) domestic wet biomass: sewage sludge, manure, industry waste, and household garbage;
 - (3) domestic plant (crops): agriculture residues.
- Nonbiogenic carbon sources, including
 - (1) fossil fuels import: NG (natural gas) and LFO (light fuel oil), diesel, gasoline, and jet-fuel (kerosene);
 - (2) domestic fuels: nonbiogenic waste;
 - (3) others: construction emission for technologies and direct cement manufacturing emission.

Coal import is not considered in this model due to the Swiss policy of phasing out coal. Table 2 summarized the domestic biomass potential for energy usage by aggregating all the corresponding subcategories listed in the biogenic carbon sources. It is highlighted that only the sustainable part of the biomass potential was integrated in Energyscope.

In addition to domestic biomass resources, biofuel import contributes to the energy supply as well. In Switzerland, all nonbiogenic energy fuels depend on import, except nonbiogenic wastes. Among the carbon sources, cement manufacturing calls for special scrutiny due to the large amount of the direct emission from $\text{CaCO}_3 \rightarrow \text{CaO} + \text{CO}_2$. Approximately 60% (Dean et al., 2011) of CO₂ emissions from cement production arise from the calcination of limestone (CaCO₃) to form CaO (the main precursor for cement production), with the remaining emissions from the process of fuel utilization for heating the kiln and effecting the clinkering reactions (Bui et al., 2018). In Energyscope, the indirect emission of cement manufacturing associated with heat supply is reckoned in industry heat demand, while the direct emission that amounts to 1.62 Mt CO₂ per year (Zuberi and Patel, 2017) is counted separately with the hypothesis of a uniform distribution over all periods.

In 2017, Switzerland generated in total 80–90 Mt waste (FOEN, 2018), of which 86% stemmed from construction

TABLE 2 | Domestic biomass potential for Switzerland, extracted from Burg et al. (2018).

	Wood	Wet biomass	Plant
Sustainable potential (GWh)	14,000	8,856	4,300
Total potential (GWh)	41,667	10,097	4,903

waste, including excavated waste (57 Mt) and deconstruction waste (17 Mt). Approximately 30% deconstruction waste went further to incineration and landfill. Additionally, 7% of the total waste is composed of the municipal solid waste (MSW), where 53% was recycled and the remaining 2.9 Mt went to incineration. The third-largest source, biogenic waste, took account of approximately 6% of the waste stock, including food waste, agricultural waste, and dry sewage sludge, etc. In order to avoid double counting the biomass, the waste in Energyscope refers to merely the nonbiogenic waste, i.e., the nonrecyclable MSW for energy usage: construction waste is not considered since it is accounted in the availability of wood; similarly, biogenic waste is incorporated into the wet biomass category. By this approach, the annual waste in 2017 amounts to 9.835 TWh, with an average LHV value of MSW 12.35 MJ/kg (Michel, 2012). We further assume an increase in waste availability by 42.8% in 2050 in correspondence to the estimation of GDP development by SECO (2020). One constraint (Eq.22) is integrated into the model reflecting the following two assumptions:

- waste generation rate is uniform over the year;
- waste can be neither accumulated nor exported, implying immediate disposal (e.g., burning in a CHP boiler) when generated.

$$F_t(\text{WASTE}) \sum_{t' \in T} t_{op}(t') = \text{avail}(\text{WASTE}), \quad (22)$$

where the *avail* represents the annual amount of waste generated within Switzerland.

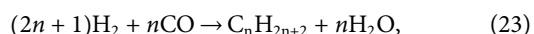
3.2.2. Carbon Conversion Technologies

Conventional boilers, oil-based vehicles are the major technologies for conversing FEC to satisfy EUD with associated efficiencies. These technologies are mature and have been discussed in numerous articles. In this section, we focus on biomass-based technologies including the following:

- Pyrolysis: The thermal cracking of wood, or solid biomass in general, in the absence of oxidizing conditions. Pyrolysis can deliver a variety of products including gaseous, liquid, and solid mixtures of organic and inorganic compounds, depending on the operating conditions. The heating rate is prevalent among them, determining the intensity of the carbon bond scission and thus, the final distribution of the product mix. Although pyrolysis is considered to be the first step of biomass gasification in order to produce a gaseous fuel, a standalone process can be utilized and targeted

toward the production of bio-crude, a liquid hydrocarbon mixture that should undergo further treatment to produce biodiesel.

- **Gasification:** Woody biomass can be converted to a gaseous fuel stream comprised mainly CO and H₂ (syngas) and to a smaller extent CO₂ and CH₄ through gasification, a thermochemical process that employs biomass oxidation in substoichiometric conditions to favor the production of CO instead of CO₂. Different oxidizing media such as steam, air, or pure oxygen directly affect the product distribution in the outlet stream. Gasification is a mature technology that uses a variety of different reactor configurations depending on the intended use of the produced syngas. Temperatures inside the gasifier can reach up to 700°C and usually, the heat is partially provided by combustion of a fraction of the product gas. Syngas from the gasifier can be used in a diverse number of ways including the focus on gaseous fuel production such as H₂ or CH₄ as well as liquid fuel synthesis. Hydrogen production is controlled by the process setup including the type and operation of the gasifier, nature of the oxidizing medium, and operating conditions such as the reactor temperature and the feed stream composition. On the other hand, production of biomethane requires a subsequent upgrade of the syngas with reaction with H₂ results in enriching the product gaseous fuel in CH₄ as CO and CO₂ are converted into methane through the Sabatier reactions.
- **Fischer–Tropsch synthesis:** The Fischer–Tropsch (FT) reaction, first developed by Franz Fischer and Hans Tropsch in the 1920s, is a catalytic synthesis process realized as polymerization of carbon atoms. It is mainly used to produce synthetic biofuels from gasification-derived syngas. The chemical reaction is described by a simple representation of the form:



where *n* is the number of carbon atoms in the polymer chain. The conversion conditions (around 200–300°C and pressure in the range of tens of bars) are used to inhibit the formation of small alkanes, but rather push toward the production of long-chain hydrocarbons with carbon chains of 10–20 atoms, according to the Anderson–Schulz–Flory (ASF) distribution. The FT process uses catalysts to promote the growth of the carbon chain, with nickel or cobalt being the most commonly used ones. However, their low poisoning resistance to sulfuric derivatives dictates stringent syngas cleaning steps prior to insertion in the FT reactor. The produced hydrocarbon blend must then undergo hydrotreatment in order to obtain the desired biofuel quality. The addition of hydrogen in a subsequent hydrocracking reactor leads to the chemical cleavage of the long-chain hydrocarbons and under controlled conditions, the acquisition of a paraffin blend (biodiesel) of the desired quality.

- **Anaerobic digestion:** Anaerobic digestion (AD) is a biochemical process that is used to break the biogenic

carbon of wet biomass and release it in the form of biogas, a gaseous mixture of CH₄ and CO₂. Digestion of wet biomass under anaerobic conditions is realized with the aid of suitable bacteria and proceeds through a complex series of (bio-)chemical reactions that can be grouped in four main stages, namely, hydrolysis, acidogenesis, acetogenesis, and methanogenesis. A set of parameters including the temperature and pH are decisive for the efficient operation of anaerobic digestion. In particular, three types of bacteria are used depending on the temperature of operation: thermophilic (45–55°C), mesophilic (25–45°C), and cryophilic (below 25°C). The production of methane is directly linked with the type of the employed bacteria and is positively affected by temperature; a direct compromise between methane production and energetic demands to sustain the operating temperature to levels above room temperature. Anaerobic digestion results also to a liquid by-product stream, the digestate, which contains all undigested biomass as well as the valuable nutrients originally in the feed stream. Due to the latter, digestate streams are mostly used nowadays as soil fertilizers. However, the high carbon content of this residual stream leaves room for additional retrieval in the form of fuels by hydrothermal treatment. The energy efficiency of anaerobic digestion greatly depends on both the nature of the digested biomass and the operating conditions. Together, they define the methane potential for each case (i.e., the produced volume of methane per mass unit of digestible matter). As the energetic content of methane is the only source of contained energy in the output biogas stream, the methane potential is a crucial parameter to define the energy efficiency of the process.

- **Hydrothermal gasification (HTG):** Hydrothermal gasification (HTG) offers the possibility of converting wet organic streams into methane using high pressure to reach supercritical water conditions in a complex reactor scheme. Compared to traditional gasification, it offers the advantage of utilizing the wet stream as it is, avoiding the preceding energy-intensive drying step. Moreover, water in its supercritical condition has a low density and dielectric constant. Consequently, it changes from polar to nonpolar solvent, and thus, the organic compounds dissolve easily in it. Furthermore, the supercritical conditions that prevail within the HTG reactor also ensure that the nitrous and phosphoric minerals contained in some forms of wet biomass such as sewage sludge and manure are released unharmed in the residual output stream. Apart from the direct processing of wet biomass streams, HTG can be used to convert the lignin-rich digestates from anaerobic digestion. On the drawbacks of the process stand the energy needed to reach the operating conditions (around the critical point of water, i.e., 370°C and 220 bars) as well as the use of a catalyst, which in turn requires special attention with regard to maintenance (poisoning prevention, degradation handling, etc.)

- **Biomass to alcohols:** Primary alcohols such as methanol and ethanol are not only individually used fuels, but also constitute chemicals used as the basis for the synthesis of higher fuels, e.g., aviation fuels. Alcohols can be produced from both woody and nonwoody biomass using different conversion pathways. Methanol can be produced from wood gasification followed by a synthesis step to convert the produced syngas. Ethanol is primarily produced via the biochemical fermentation of biomass crops such as corn, wheat, or sugarcane. Fermentation is usually preceded by pretreatment and handling steps such as milling and hydrolysis, which aims to isolate the sugars from the biomass matrix. Then, the biological degradation step is able to transform the sugars in chemicals of fuels such as ethanol depending on the design of the process.

3.2.3. Carbon Sinks

Two categories of carbon sinks are considered in Energyscope:

- **natural carbon sinks:** Biomass is regarded as a carbon sink in the process of biogenic formation. As presented, it serves also as a carbon source by combustion.
- **artificial carbon sinks:** CCUS, where the three processes, CC (carbon capture), CCS (carbon sequestration), and CCU (carbon utilization) are treated separately. Carbon capture occurs previously to the sequestration and utilization. The captured carbon has to be either stored or used.

In terms of CC process, two categories are distinguished according to their application fields: one is from large point sources with high CO₂ concentration where “conventional” carbon capture technologies could be deployed on large scales, such as a gas power plant, or a cement factory, etc. Three typical technologies are commonly applied in this category for mitigating the carbon emission, namely,

- **postcombustion:** One of the most relatively mature technologies for carbon capture. It applies to almost all industrial sectors, typically gas/coal power stations and heavy manufacturing plants. Carbon dioxide is captured from flue gases after combustion of fossil fuel at power stations or other large point sources. Postcombustion capture is most popular in research because existing fossil fuel power plants can be retrofitted to include CCS technology in this configuration (Sumida et al., 2012).
- **precombustion:** This applies to the majority of biofuels and chemical industry. There are several advantages and disadvantages compared to conventional postcombustion CC. The CO₂ is removed after the combustion of fossil fuels, but before the flue gas is expanded to atmospheric pressure. The capture before expansion, i.e., from pressurized gas, is standard in almost all industrial CO₂ capture processes, at the same scale as required for power plants (Bryngelsson and Westermark, 2009; Starr, 2009).
- **oxy-fuel:** The fuel is burned in oxygen instead of air in order to obtain an almost pure carbon dioxide stream that can be transported to the sequestration site or reused. The cement

industry is considered one of the most promising application fields for deploying this technology.

By contrast, the other category of CC process is specified for the nonconcentrated carbon emission, typically involving transportation (including aviation) and other fugitive emissions, e.g., the emission to the atmosphere due to incomplete absorption/adsorption of conventional carbon capture technologies. These emissions are not supposed to be capturable except via natural carbon sinks (biomass) or DAC (direct air capture). As an emerging technology, the latter is commonly as much as 3–5 times that of conventional CC technologies.

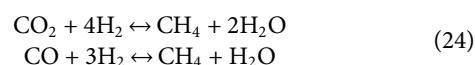
Following carbon capture, either CCS or CCU should be applied. Carbon storage implies depositing the captured CO₂ into an underground formation for preventing release into the atmosphere in a long period, typically hundreds or thousands of years. According to the geological and geographical analysis conducted by Chevalier et al. (2010), Switzerland has a CCS potential in aquifer amounting to 2.7 billion tons that is approximately 67 times compared to the current anthropogenic emission 47.24 Mt/year (Stadler et al., 2019).

Different from carbon storage, carbon utilization consists in making use of the captured CO₂ to produce fuels or chemical products, such as methane, methanol, and ethylene. In these cases, CO₂ serves as a necessary raw material for production. Despite the relatively high cost compared to CCS, carbon utilization facilitates energy systems’ coupling in transferring CO₂ among sectors as intermediate energy carriers. This feature, together with e-hydrogen (stemming from electrolysis), is promising in alleviating the increasing intermittency from massive penetration of renewables. The following section will present several typical CCU processes and their roles in the energy transition.

3.2.4. CO₂-to-X

In the context of the energy system decarbonization, CO₂ can be treated as a carbon source, an input material for the production of synthetic fuels and products. This is realized through a number of considered CO₂-to-X processing technologies, able to transform CO₂ to valuable outputs. The main considered CO₂-to-X technologies are listed below:

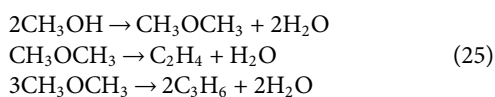
- **Methanation:** Methanation is a catalytic conversion process through which, CO₂ reacts with H₂ in order to produce synthetic methane. Methanation is often referred to as the Sabatier process and is described by the following chemical reactions:



Methanation requires moderate temperatures (in the range of 250C–350°C) and pressures as high as 20–25 bars. As the reaction makes use of a catalyst to aid with the conversion, the latter usually being nickel or cobalt, it is evident that the input streams

must be rid of any impurities such as sulfur and hydrocarbons that could poison the catalyst either by deactivation or by coke deposit.

- **CO₂-to-diesel:** Biodiesel, being a blend of mainly linear hydrocarbons, can be mainly produced through Fischer–Tropsch synthesis using a carbon source and hydrogen. In the examined case, captured CO₂ undergoes a shift reaction in order to create an input stream compatible with the prerequisites of the mainstream FT catalysts in terms of H/C ratio and is then inserted to the FT reactor along with a hydrogen-rich stream. As the origin of the utilized hydrogen plays no part in the operation of this particular process, it is assumed to be taken as a product from other processes such as water electrolysis.
- **CO₂-to-jet-fuel:** In a process similar to the above, captured CO₂ is used to synthesize a fuel blend through Fischer–Tropsch synthesis. Using appropriate composition tailoring of the produced mixture as well as subsequent fuel upgrading, a liquid blend similar to jet-fuels can be obtained. The bio-jet-fuel blend is assumed to be able to be used as a substitute for conventional fossil jet-fuels.
- **CO₂-to-methanol-to-X:** Methanol is one of the key chemical compounds, not only due to its use as a standalone chemical, but also its further application as a material for synthesizing other chemicals. It is thermochemically produced from CO₂ hydrogenation in a process that is similar to biodiesel synthesis. Methanol can be then further processed to give a variety of different useful chemicals. Low carbon chain olefins such as ethylene and propylene can be produced by catalytic conversion of methanol via dimethyl ether (DME) in a process known as methanol to olefins (MTO), which follows the following reaction scheme:



Both ethylene and propylene constitute chemicals that mainly represent building blocks for subsequent synthesis of polymers widely used in the plastics industry, namely, polyethylene and polypropylene, respectively, or raw materials for the production of other chemicals such as acetic acid. In this study, acetic acid can be either produced through either ethylene cracking or more directly, from carbonylation of methanol. Methanol itself can also be transformed into a mixture of aromatics, mostly benzene and toluene as well as a blend of xylenes (dominated by *o*- and *p*-xylene). The latter conversion process serves as a method of synthesizing the aforementioned aromatics directly from captured CO₂, despite its low energy yields due to various processing steps.

3.2.5. Carbon Flows

As stated, carbon flows with in-depth penetration of biomass and CO₂-to-X technologies are complicated in the presence of interconnected loops. **Figure 2** depicts the conceptual carbon

flows in the system, where carbon sources are divided into biogenic and nonbiogenic parts:

- biogenic carbon inputs lead to at maximal net-zero emission; negative emission could be realized in the presence of BECCS.
- nonbiogenic carbon inputs result in at least net-zero emission. In reality, it is impossible to realize 100% carbon capture and as a result, nonbiogenic carbon emission keeps always positive.

In Energyscope, the carbon balance is handled by the CO₂ layers that behave as tanks with incoming carbon flows from various sources and outgoing flows to different locations. The following list summarizes the CO₂ layers defined in the MILP model:

- **CO_{2A}:** the carbon emission from carbon-intensive fields. This amount of carbon emission is capturable by applying conventional carbon capture technologies. In Energyscope, emissions from centralized thermal plants are computed into this category.
- **CO_{2C}:** the captured carbon, which is assumed to either be used or stored later; in this level, CO₂ storage could be further categorized as:
 - **CO_{2S}:** sequestration, where the CO₂ is buried into underground formation and cannot be reused;
 - **CO_{2SS}:** temporary storage, implying the CO₂ is capable of being used later.
- **CO_{2E}:** in contrast to CO_{2A}, the CO_{2E} refers to the carbon emission from nonconcentrated spot sources, e.g., a car or a household wood furnace. In addition, it includes the fugitive emission in conventional carbon capture processes, as well as the emission from construction periods. These emissions are not supposed to be mitigated without biomass photosynthesis or direct air capture (DAC). In Energyscope, all emissions stemming from decentralized (DEC) technologies belong to this category.

Figure 2 illustrates the relationship of the CO₂ layers defined in the model. All technologies are linked to one or more CO₂ layer(s) with corresponding emission factors. Through this approach, each technology in Energyscope emits or absorbs certain amount of CO₂ from corresponding layers, leading to the net emission in each period *t* expressed by:

$$\begin{aligned} \text{Emission}(t) &= \sum_{j \in \mathcal{E}, c \in \mathcal{C}} \mathbf{F}_t(j) t_{op}(t) \eta(j, c) \quad \forall t \in \mathcal{T} \\ \sum_{t \in \mathcal{T}: t \leq t'} \text{Emission}(t) &\leq \epsilon \quad \forall t' \in \mathcal{T}, \end{aligned} \quad (26)$$

where \mathcal{T} represents the set of periods, and \mathcal{C} denotes the carbon layers of CO_{2A} and CO_{2E} covering both concentrated and dispersed carbon emissions. η denotes the emission factor with unit ktCO₂/GWh for the technology *j* in a certain layer *c*. Instead of limiting merely the annual emission, a more strict ϵ -control is

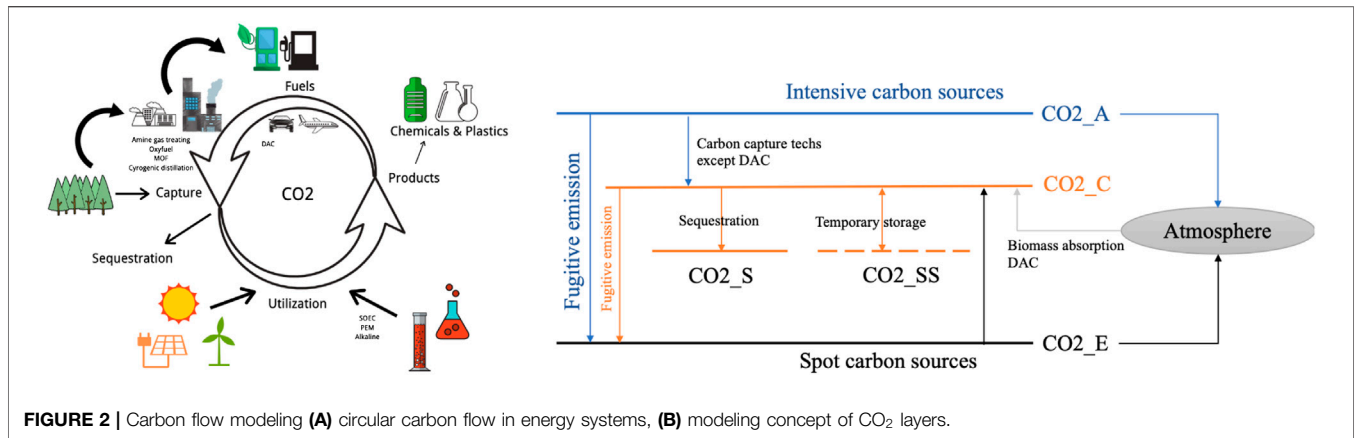


FIGURE 2 | Carbon flow modeling (A) circular carbon flow in energy systems, (B) modeling concept of CO₂ layers.

introduced to ensure that the total emission levels within all periods previous to t' ($t' \in \mathcal{T}$) do not reach the limit set by ϵ .

As illustrated in the **Figure 2B**, the captured CO₂ (CO_{2C}) can either be transformed to fuels and chemical products, or be stored temporarily or permanently (sequestered underground). This concept is translated into **Eq. 27**:

$$\sum_{j \in CC} F_t(j) = \sum_{j \in CCS} F_t(j) + \sum_{j \in CCU} F_t(j) + \sum_{j \in CTS_{in}} F_t(j) - \sum_{j \in CTS_{out}} F_t(j) \quad \forall t \in \mathcal{T} \tag{27}$$

which reflects the carbon balance of carbon sources and sinks, where the inputs stem from all carbon capture technologies CC , and the outputs flow to CCS and CCU , representing all the carbon sequestration and utilization technologies, respectively. Specifically, the cost for a given CC or CCS technology $c(j)$ is expressed as Swiss franc per ton of CO₂ captured or sequestered. This practice takes into account the whole lifespan of a technology into consideration. Therefore, the annual cost of a given CC or CCS technology j could be expressed by **Eq. 28**:

$$c(j) \sum_{t \in \mathcal{T}} F_t(j) t_{op}(t) \quad \forall j \in CC \cup CCS, \tag{28}$$

where F_t is of unit kt-CO₂ captured per hour.

4. HISTORICAL DATA AND ASSUMPTIONS ON SWISS ENERGY SYSTEM

4.1. Demand

Figure 3 illustrates the historical EUD in Switzerland and defines three scenarios according to **JASM (2020)**: scenario REF representing the base scenario; scenarios HIGH and LOW depicting the high- and low-energy demands in respective sectors. This article adopts the scenario REF as the base scenario for analysis.

Additionally, plastics and chemicals demands are integrated into EUD (**Figure 4**) in order to have a holistic view on the carbon flow chains. It is assumed that the demands for chemicals and plastics in 2050 keep the same as 2017 due to a trade-off between increasing population and recycling rate. Intermediate products

include ethane, ethylbenzene, benzene, propylene, ethylene, styrene, p-xylene, and toluene.

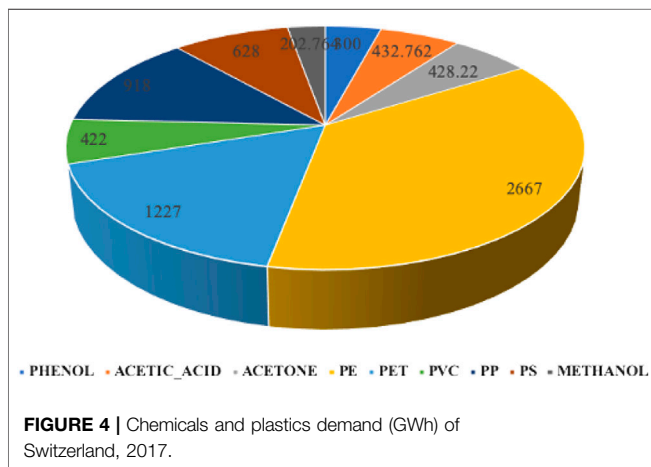
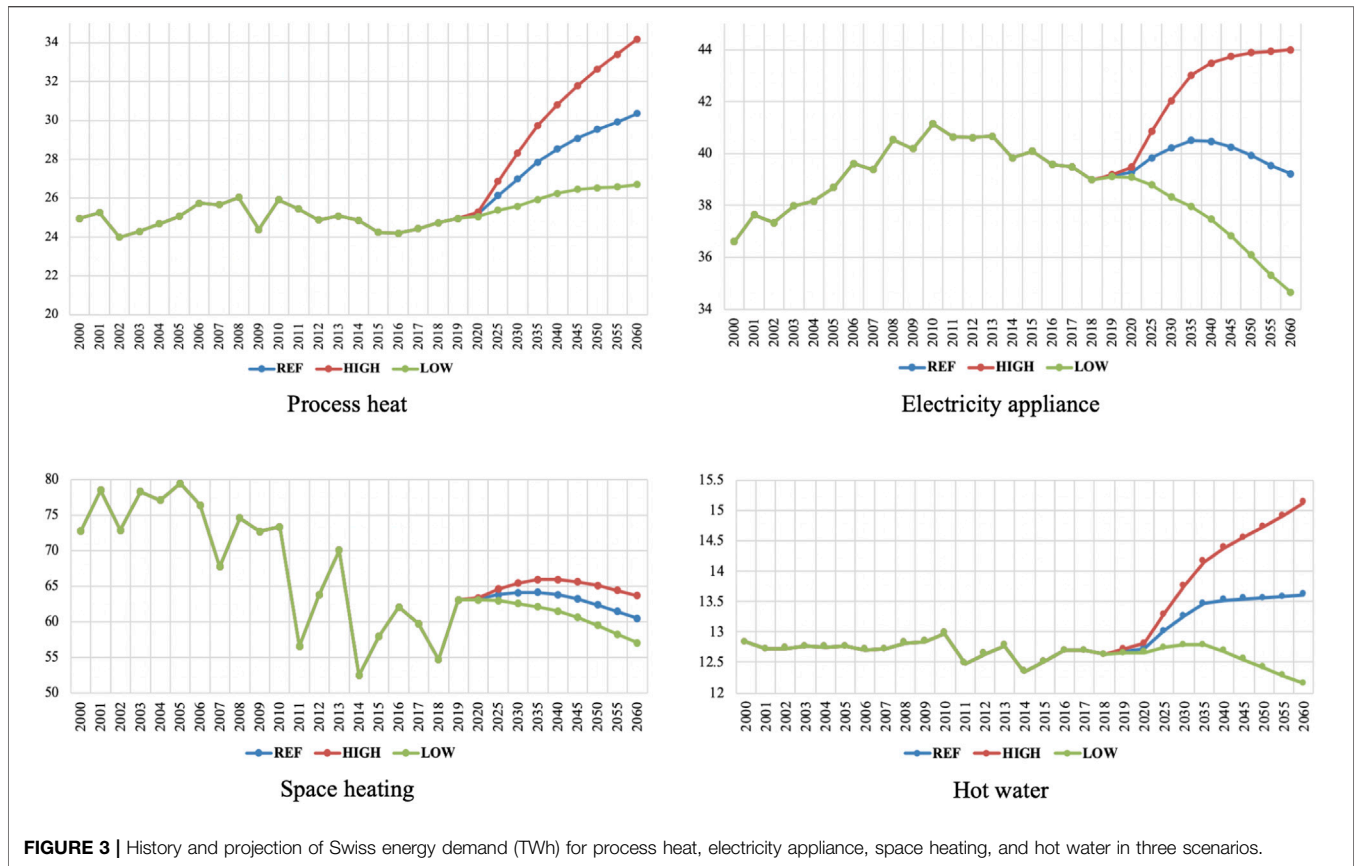
Transportation accounts for more than 1/3 of final energy consumption in the current Swiss system. The passenger and freight demand (excluding aviation) in 2050 are estimated to be 140,300 Mpkm (million passenger kilometer) and 39,700 Mtkm (million ton kilometer), respectively (Stadler et al., 2019). In terms of aviation, we distinguish the short-distance and long-distance flight, and estimate the demand via **Eq. 29**:

$$\sum_{i \in \mathcal{F}, j \in \mathcal{C}} r(i)f(i, j), \tag{29}$$

where the r represents the share of flight category for short distance (within Europe) and long distance (outside Europe) in the flight set \mathcal{F} . The f indicates the conversion factor of energy consumption (unit MJ) with respect to 1 pkm EUD in different classes \mathcal{C} (economy, business, and first class) for short- and long-distance aviation, respectively. This approach results in the specific weighted energy consumption for Swiss aviation: 2.1226 MJ/pkm, translated to 22.6 TWh kerosene equivalent (see **Supplementary Material**). This value corresponds well to the amount of kerosene consumption 21.4 TWh/y reported by Stadler et al. (2019). By taking a projection factor of 1.33 in 2050 compared to 2015 defined in Commission européenne and Direction générale de la mobilité et des transports (2016), the passenger aviation demand is estimated to be 50,800 Mpkm in 2050.

4.2. Current Energy Mix

As a country lacking fossil fuels, the current energy supply of Switzerland depends predominantly on imports. Petroleum products and natural gas accounted for approximately 60% in the energy mix. In the power sector, hydro power dominated with around 50% share, and wind and PV were developing rapidly [PV production in 2018 was roughly 40 times the value in 2008 according to BFE (2018a)]. First, we applied Energyscope on the energy system of Switzerland in 2017 for calibration. From the corresponding results shown in **Figure 5**, the renewable penetration accounted for around 30% in the Swiss FEC mix, associated with carbon emissions from fossil and nonfossil fuels 40.7 and 10.0 Mt/y, respectively.



5. DECARBONIZATION SCENARIOS

5.1. Scenario Definition

This section focuses on two issues: 1) Is it possible to realize carbon neutrality in 2050 for Switzerland? 2) If yes, what does the optimal energy system look like? First, the ϵ value of CO₂ limit is fixed to zero in Eq. 26, and second, two scenarios are defined:

- scenario a: allowing the utilization of fossil fuels
- scenario b: banning the utilization of fossil fuels

Additionally, electricity import is prohibited within both scenarios in order to realize power autonomy. The availability for wood, wet biomass, and plants (crops) follow the definition in Table 2. PV potential varies in literature: according to SFOE (2019), Swiss roofs and facades have the potential to generate 67 TWh of electricity per year, where 50 TWh is estimated from roofs larger than 10 m², and 17 TWh from walls for at least 20 m² average exposure to excellent sunlights with hypothesis that 45–60% of their surfaces can be covered with PV panels. Assouline et al. (2016) indicated the PV power production for urban areas in Switzerland in 2050 was expected to reach about 32 TWh. In this article, the maximal installed capacity of PV panels in Switzerland in 2050 is set to be 40 GW. Compared to the solar energy, the development potential for wind is limited and estimated to be 4.4 GW (BFE, 2018b) in 2050. Table 3 lists the key assumptions in the scenarios.

In Energyscope, imported resources are regarded as nonstorable due to techno-economic consideration, implying “import only when needed”. Domestic fuel products, such as hydrogen from electrolysis, are assumed to be storable. In the following paragraphs, the results of scenarios a and b are analyzed, respectively, with further discussion in Section 5.3.

5.2. Results

5.2.1. Net-Zero Emission With Fossil Fuels

The Sankey diagram in Figure 6 illustrates the optimal carbon flows of the considered energy system with fossil fuel utilization.

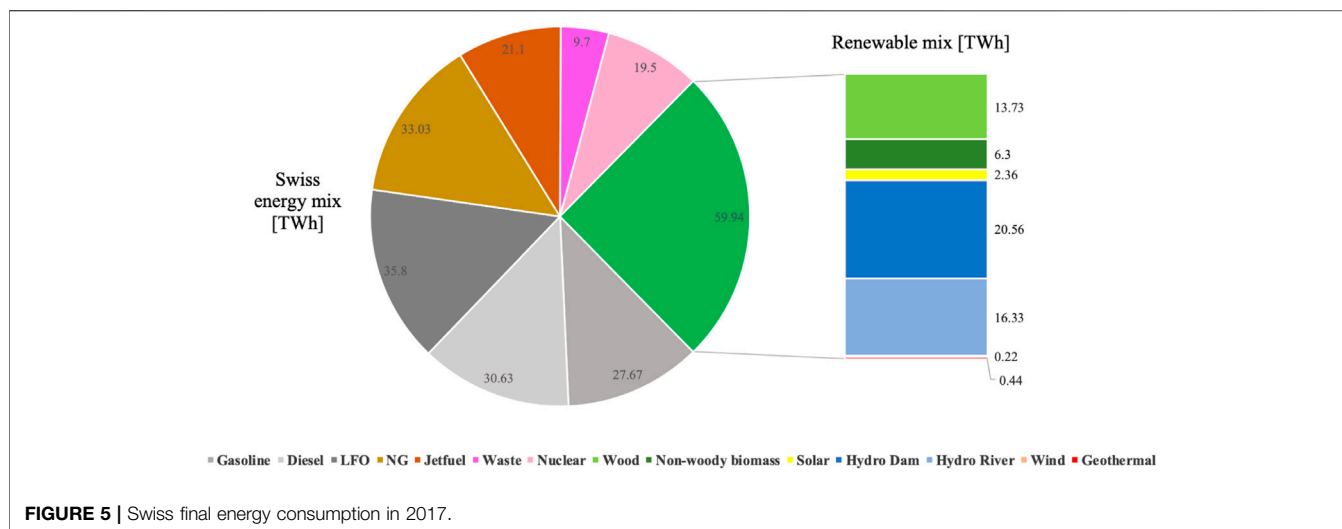


FIGURE 5 | Swiss final energy consumption in 2017.

TABLE 3 | Assumptions in Energyscope.

Parameter	Range		Note
	Min	Max	
Public mobility share in passenger transportation	21%	50%	The min is set to the value in 2017
Train ratio in freight transportation	37%	80%	The min is set to the value in 2017
Share of (bio) gasoline and (bio) diesel vehicles	20%	100%	The min value is based upon experts' opinion
District heating share in low-temperature heat supply	5%	70%	The min is set to the value in 2017
District heating loss	5%	5%	According to Moret (2017)
Geothermal share in district heating	0%	30%	Assumption
Transmission and distribution power loss	7%	7%	According to SFOE (2015)

The width of the arrow is proportional to the amount of carbon flow expressed as kt of C element per year. For instance, a part of CO₂ (CO₂E) in the atmosphere is captured by wood and then converted to diesel via FT (Fischer–Tropsch) process, which is further converted into CO₂ again after combustion in a truck engine, and is released back to the atmosphere, thus forming a closed loop that represents a complete carbon flow chain. In this figure, DHN, DEC, and IND represent district heating, decentralized technologies, and industrial energy supply technologies, respectively.

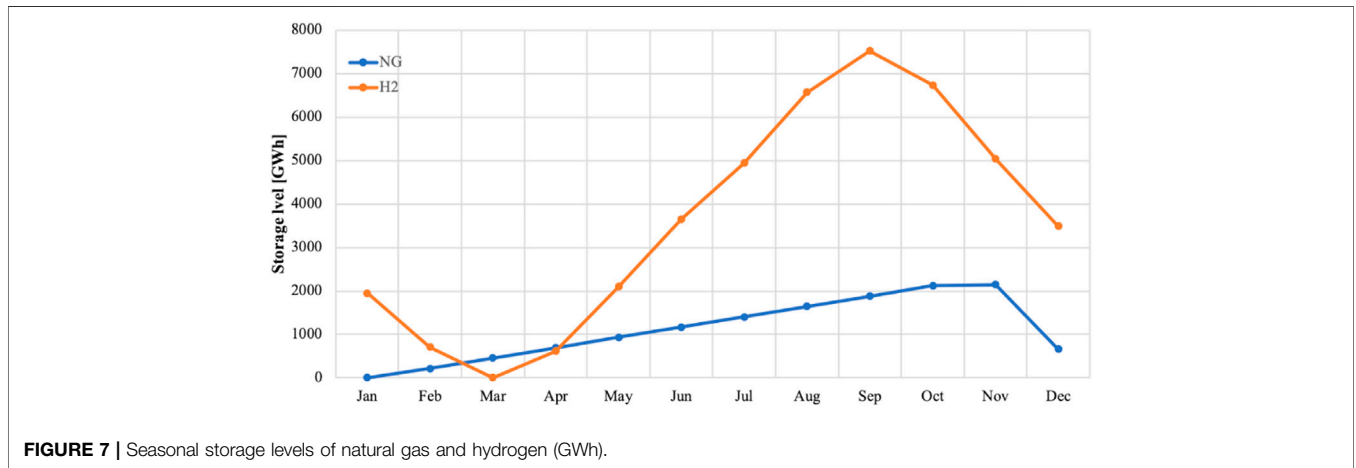
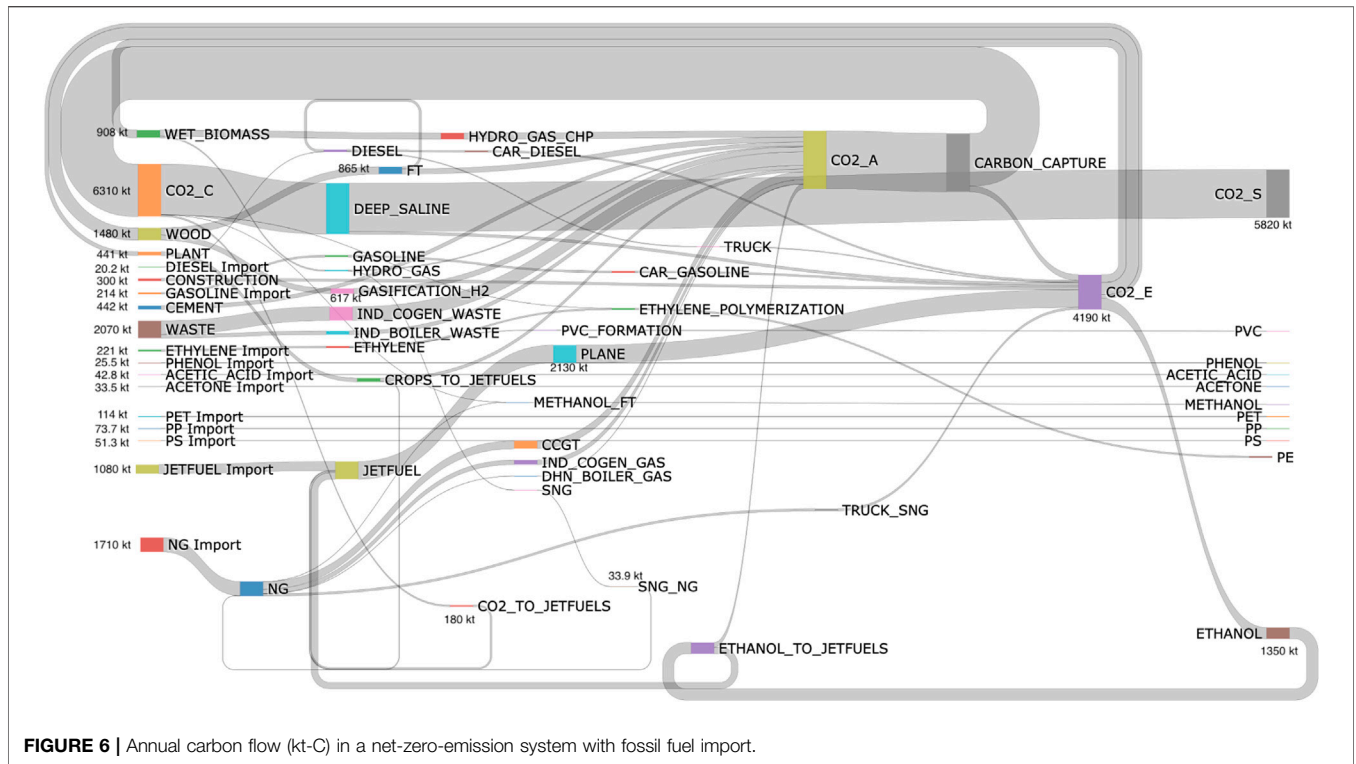
In terms of nonbiogenic carbon, natural gas import in this scenario amounts to 31.64 TWh/y, approximately the same level as today (33 TWh): the majority (84%) is used for power and heat supply, while 15% serves for transportation and the remaining part is transformed to methanol. Nonbiogenic waste is predominantly incinerated in combined heat and power plants. As the most important energy carriers, the two sources contribute to 3,780 kt-C/y. Other nonbiogenic carbon sources stem mainly from jet-fuel (excluding the biogenic part coming from ethanol upgrading), construction, and cement industry, as well as a small part of gasoline and diesel. The significant drop in fuel consumption results principally from deep electrification in the mobility sector. As for biogenic carbon, the saturation of domestic biomass sustainability is witnessed, translated to 2,829 kt-C/y contributing 27.2 TWh/y to the energy system.

Wood is largely converted to hydrogen and diesel, while wet biomass is all consumed by hydrothermal gasification for producing synthetic natural gas. Plants are in majority converted to jet-fuel (441 kt-C/y) via fermentation processes.

Based upon the optimization results, chemicals and plastics depend mainly on import, except PVC, PE, and methanol, which could be synthesized from intermediate materials. 3% of the captured carbon (CO₂C) participates in the formation of chemicals/fuels/plastics with the remaining 97% being sequestered underground. The results suggest that carbon neutrality for Switzerland in 2050 is theoretically feasible by exploiting domestic biomass up to its limit and deploying considerable CCS (5,820 kt-C) in order to offset nonbiogenic emissions. Neither natural gas storage nor hydrogen storage is observed in this case due to a higher cost of domestic synthesis compared to imports.

5.2.2. Net-Zero Emission Without Fossil Fuels

Scenario b aims at decarbonizing the energy system without importing fossil fuels. Similarly, biomass is fully exploited and the majority of biogenic carbon is converted to biogas and liquid biofuels. Waste serves as a major source for nonbiogenic carbon. With regard to the carbon sinks, CCS declines to 3,744 kt-C/y from 5,820 kt-C/y in scenario a, while CCU climbs due to the production of diesel (766 kt-C/y) and jet-fuel 663 kt-C/y, as well



as plastics (8 kt-C/y). The results demonstrate the dominance of CCS as the major negative emission technology and the principal role of CCU as clean fuel supplier.

In **Figure 9**, the annual natural gas storage level is represented via the loop NG → NG_STO → NG, where hydrogen storage is not included due to its zero carbon content. Furthermore, **Figure 7** depicts the monthly storage variation of both natural gas and hydrogen, where a continuous increase of hydrogen level is observed from March to September, after which the system starts to discharge. Similarly, natural gas storage begins in February and assumes the maximum in October. This trend corresponds well to the reverse-seasonality of PV production and energy demands: in summer, the energy surplus reaches the peak

where the maximal storage level amounts to 10 TWh. As to the monthly variation of CO₂ storage level shown in **Figure 8**, the peak and the trough appear in winter and summer, respectively, in correspondence to the distribution of energy demand intensity of Switzerland.

Based upon the modeling results, a massive penetration of renewables is obligatory for realizing carbon neutrality: **Figure 10** reflects the output of renewable technologies (positive value) as well as electrolysis (negative value). Biomass is not included here since it is mainly used for fuel production as discussed previously. An obvious positive correlation is observed between electrolysis and the renewable power outputs, especially the intermittent renewables (PV and wind). Hydropower accounts for nearly

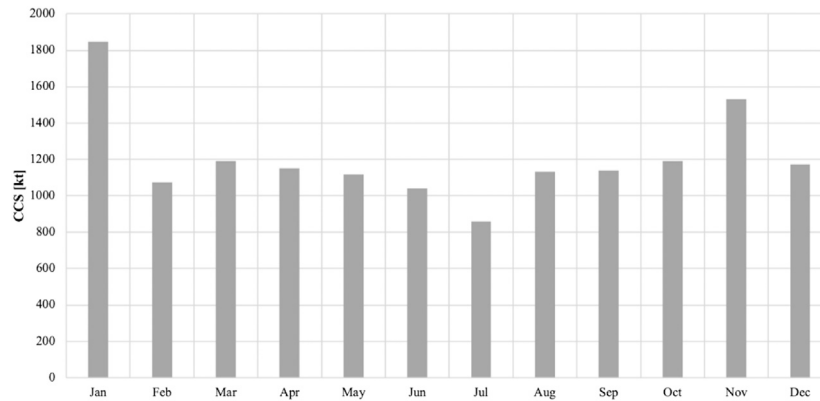


FIGURE 8 | Monthly carbon sequestration (kt-CO₂).

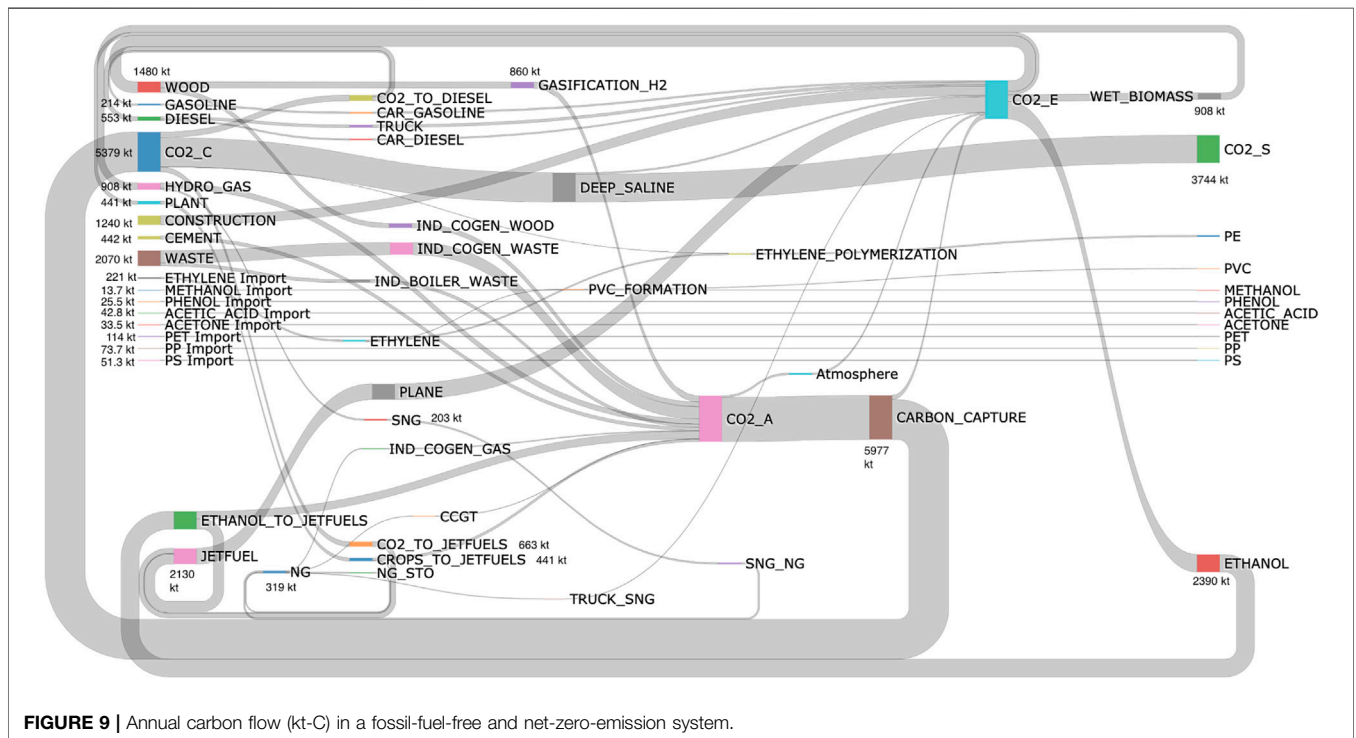


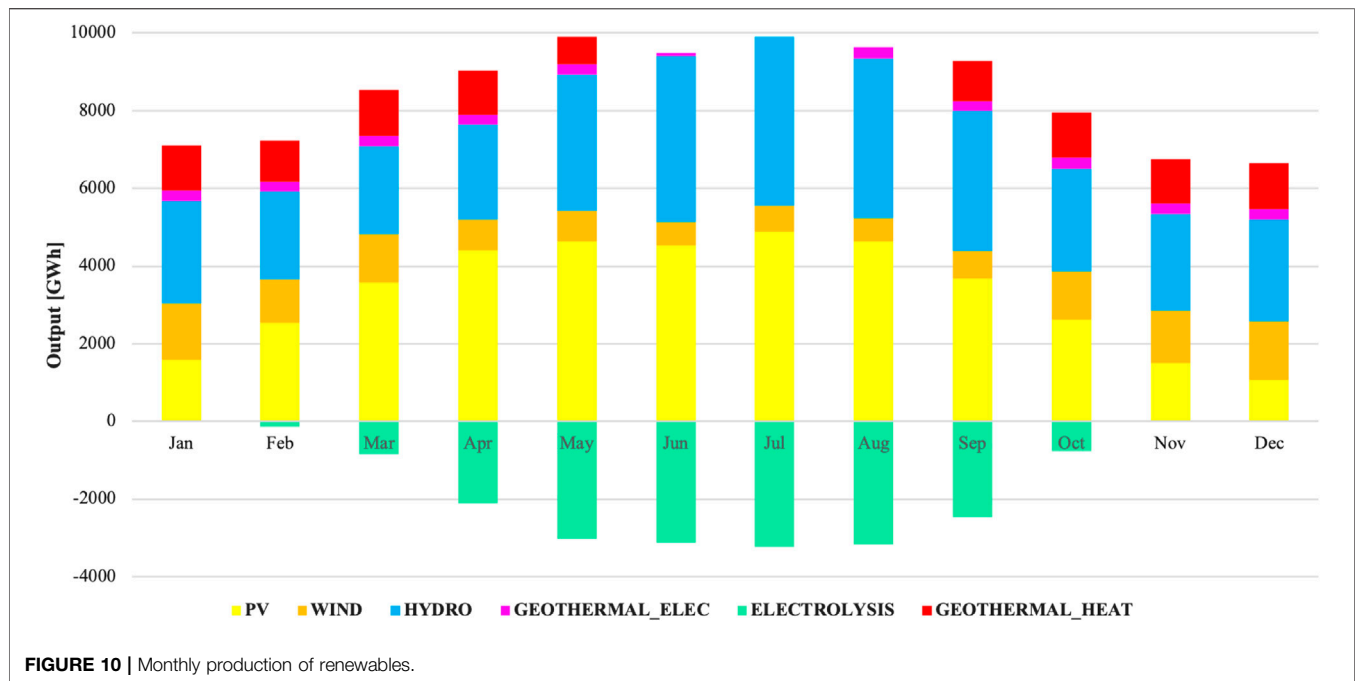
FIGURE 9 | Annual carbon flow (kt-C) in a fossil-fuel-free and net-zero-emission system.

half of the total renewable outputs and is distributed relatively uniformly among the months. In summer, PV and hydro contribute approximately the same amount of power to the system. Geothermal is predominantly used for heat supply in cold seasons.

5.3. Discussion

Table 4 summarizes the key findings on the carbon flows from the two scenarios. In the presence of fossil fuels, CCS is deployed on a large scale with limited CCU due to the relatively lower cost of imports than domestic production. Phasing out fossil fuels results in an explicit increase for CCU and a decline for CCS as a result of the deficit for fuels. CCU is capable of shifting emissions

among different technologies and in different periods due to seasonal storage, which is yet not able to directly mitigate the anthropogenic carbon emission by nature, except the small part in plastics synthesis. However, CCU results in a steep decline of nonbiogenic carbon entering the energy system by providing alternative e-fuels and biofuels. From this perspective, all the carbon emissions stem originally from “above the ground” and circulate internally, implying no carbon accumulation in the energy system. Despite an increase of the total cost around 3.3 billion CHF/y, scenario b is considered more radical in terms of realizing fossil-free society and diminishing the overdependence on CCS, which may result in unexpected geologic impacts. It should be highlighted that the total cost of

**TABLE 4 |** Scenario comparison.

	Scenario a	Scenario b
Total cost (MCHF/y)	25,152	28,451
Net carbon emission (kt-C/y)	0	0
Biogenic carbon inputs (kt-C/y)	4,179	5,219
Wood	1,480	1,480
Wet biomass	908	908
Plant (crops)	441	441
Ethanol import	1,350	2,390
Nonbiogenic carbon inputs (kt-C/y)	6,390.5	4,327.5
Fuel/construction/cement ^a	5,828.7	3,752
Chemicals/plastics	561.8	575.5
Carbon capture (kt-C/y) ^b	6,310	5,379
Carbon sequestration (kt-C/y)	5,820	3,744
Fugitive emission (kt-C/y)	301.3	198
Carbon utilization (kt-C/y)	188.7	1,437
Fuel	180	1,429
Chemicals/plastics ^c	8.7	8

^aEmission in cement manufacturing stemming from fuels not included.

^bIncluding biogenic and nonbiogenic CC.

^cProcesses without direct participation of CO₂ are not included in CCU.

the energy system is of large uncertainty depending predominantly on the specific investment and operational costs for the considered resources and technologies, which was discussed in the previous studies (Moret et al., 2017; Li et al., 2019). The results in this article are based upon the EUD projection in 4.1, which could be further reduced by energy efficiency improvement, for instance, building renovation and innovative industrial process design, as well as lifestyle change, such as substitution of private cars by increasing bicycles. All these effective measures contribute to the acceleration of the decarbonization process and by consequence, reinforcing the plausibility of the realization of carbon neutrality illustrated in this study.

Concerning the limitations of this research: The infrastructures in the energy system are not fully modeled, e.g., the pipelines for hydrogen. In addition, the emission factors for each technology during construction in the future are based upon the present values that are supposed to decline due to the intensification of carbon mitigation. In terms of CCS, this model reports the amount of CO₂ needed to be sequestered, but no further information on where to store and how to transport the CO₂ from sources to sinks. Therefore, it requires industrial pilot projects for further demonstration and benchmarking; in particular the development of biomass and CCUS technologies as well as auxiliary infrastructures.

6. CONCLUSION

This article comes up with a systematic methodology of modeling carbon flows in a complex energy system in favor of sustainable strategy decisions for the long-term energy transition toward a carbon-neutral society. It proposes an optimization approach for solving the complex carbon loop issues emerging from the massive penetration of renewables and CCUS technologies. Results demonstrate that a radical reformulation of the current energy system is obligatory, where the participation of biomass is indispensable. By quantifying the carbon flows among various sources and sinks, this article depicts the optimal configurations of the Swiss energy system in terms of techno-economic consideration, concluding the following:

- for nonbiogenic carbon: CCS serves as an absolute carbon sink in offsetting the nonbiogenic carbon inputs;
- for biogenic carbon: CCU with biogenic carbon sources strengthens the coupling of the whole system via power-to-X and energy storage, with net-zero (even negative) carbon emission.

In terms of Switzerland, biomass-based plants, waste incineration, and cement industry are the key areas for the deployment of carbon capture technologies. Although the applied case study is based on Switzerland, the modeling approach presented by this article is generic and applicable to different energy systems of different scales.

DATA AVAILABILITY STATEMENT

The original contributions presented in the study are included in the article/**Supplementary Material**, and further inquiries can be directed to the corresponding author.

AUTHOR CONTRIBUTIONS

XL for modeling, results analysis, and writing. TD for data management. SM for initial conceptual development of the modelling framework. The others for data collection and review.

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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.2020.549615/full#supplementary-material>

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Conflict of Interest: The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

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