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Towards Net Zero Greenhouse Gas Emissions in the Energy and Chemical Sectors in Switzerland and Beyond – A Review

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Abstract: In today's societies, climate-damaging and finite fossil resources such as oil and natural gas serve a dual purpose as energy source and as carbon source for chemicals and plastics. To respond to the finite availability and to meet international climate goals, a change to a renewable energy and raw material basis is inevitable and represents a highly complex task. In this review, we assess possible technology paths for Switzerland to reach these goals. First, we provide an overview of Switzerland's current energy demand and discuss possible renewable technologies as well as proposed scenarios to defossilize the current energy system. In here, electric vehicles and heat pumps are key technologies, whereas mainly photovoltaics replace nuclear power to deliver clean electricity. The production of chemicals also consumes fossil resources and for Switzerland, the oil demand for imported domestically used chemicals and plastics corresponds to around 20% of the current energetic oil demand. Thus, we additionally summarize technologies and visions for a sustainable chemical sector based on the renewable carbon sources biomass, CO₂ and recycled plastic. As biomass is the most versatile renewable energy and carbon source, although with a limited availability, aspects and proposed strategies for an optimal use are discussed.

Keywords: Biomass \cdot Carbon capture and usage or storage CCUS \cdot Final energy demand \cdot Net-zero GHG emissions \cdot Renewable carbon



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1. Introduction

In today's societies, fossil raw materials such as oil, natural gas and coal serve a dual purpose as energy sources and as the main carbon sources for the indispensable organic chemicals and materials fulfilling a plethora of functions in our daily life. The problems associated with the current dependence on fossil feedstocks are well-known: The combustion of fossil resources increases the concentration of the greenhouse gas (GHG) carbon dioxide (CO₂) in the atmosphere, with CO₂ being responsible for about two thirds of the currently observed global temperature increase.[1] Moreover, oil and natural gas are finite resources that will be depleted in the next few decades. Both issues are exacerbated by the increase in the global population and the standard of living in developing and emerging countries and the associated rise in energy demand. A switch to a renewable and environmentally compatible raw material base is therefore inevitable and is a global, highly complex and urgent task. Switzerland has also committed itself to the Paris Climate Agreement and with this to halving its GHG emissions by 2030 compared to 1990 levels and to take adequate measures to limit the global average temperature increase to well below 2 °C and if possible to 1.5 °C. Thus, a Federal Council resolution declared the goal to achieve net zero emissions by 2050. In addition, following the reactor disaster in Fukushima, Switzerland decided to gradually phase out nuclear energy, which makes the former goal even more ambitious. As of 2019, Switzerland has managed to reduce its domestic GHG emissions (without international aviation) from 54 Mt CO₂eq in 1990 to 46 Mt CO₂eq (-8 Mt CO₂eq, -15%). To reach the intermediate goal of 50% GHG emission reduction until 2030 (i.e. 27 Mt CO₂eq), a further reduction of 19 Mt CO₂eq in just 11 years must be achieved, albeit not necessarily only with domestic measures. According to predictions by the Swiss Federal Office of Energy, domestic GHG emissions are expected to decrease only to 40 Mt CO₂eq in 2030 and further to 32 Mt CO₂eq in 2050 with the current measures already in place.^[2] This underpins the urgent need to install further actions to reach the goal of GHG neutrality by 2050 and to move beyond theoretical pledges.

In this review, we assess possible technology paths to reach GHG neutrality in the energy and in the chemical sectors, with a focus on the situation in Switzerland. To deduce possible ways to defossilize the current energy system, the scale and the current characteristics of the main energy services that need to be transformed must be known. Thus, in this article we first give an overview of Switzerland's main drivers of the current final energy demand and discuss the possible renewable technologies and selected scenarios to defossilize today's energy system including carbon capture and storage (CCS) as an integral part. As fossil resources also serve as feedstock for imported organic chemicals and plastics, we provide an estimation of the oil consumption for this purpose and introduce production technologies and future visons for a sustainable chemical industry based on the three principle renewable carbon sources biomass, CO₂ and recycled plastic waste. As biomass is the most versatile renewable energy and carbon source, although with a limited availability, aspects and proposed strategies for an optimal use are discussed.

2. Current Final Energy Demand in Switzerland

According to the energy statistics of the Swiss Federal Office of Energy, Switzerland's final energy demand in 2019 amounted to 834 PJ (*i.e.* 834 · 10¹⁵ J).^[3] The dominant energy carriers for this are oil (407 PJ, 49%), electricity (206 PJ, 25%) and natural gas (119 PJ, 14%). Bioenergy (wood, biogenic fraction of municipal and industrial waste, biogas and biofuels) and renewable heat (environmental, solar and geothermal heat) together contribute 86 PJ (10%) (Fig. 1a).

The main drivers of the final energy demand are heat supply (362 PJ, 43%), the transport sector including international flights departing in Switzerland (314 PJ, 38%) and electricity for other purposes than heat and transport (149 PJ, 18%) (Fig. 1b). [4] In the following, the main technologies and energy sources for these purposes are summarized.

2.1 Current Technologies and Energy Sources for Heat Supply

Heat is used to temperate buildings, to make hot water and to drive industrial processes *e.g.* by supplying steam. Today, the combustion of fossil fuels (oil, natural gas, and the fossil fraction of municipal and industrial waste) is with a share of 65% the main technology to provide heat. 47 PJ (13%) of heat each are contributed by biogenic combustibles (wood, biogas, and the biogenic fraction of municipal and industrial waste) and by electricity. Burning of these fuels takes place in furnaces of different scales, in boilers to provide steam, or in combined heat and power (CHP) plants. Further renewable heat (environmental heat extracted by heat pumps and solar heat) contributes with 21 PJ a minor share to the current heat demand. (Fig. 2a).

The selection of the right technology depends among other criteria on the desired temperature level of the heat. Space heating (i.e. heating of buildings) and hot water production, accounting for 74% of total heat consumption, are typical low-temperature heat (<100 °C) applications, which can be provided by all common technologies. However, combustion provides much higher temperature levels than are actually needed. In contrast, process heat mainly requires medium (100–600 °C, 39% of all process heat) and high (>600 °C, 35%) temperature levels, for which heat pumps or solar panels are less suited and burning of fuels is often necessary.

2.2 Current Energy Sources for Transport

The transport sector, which includes passenger and freight transport by road, rail, ship and air, currently shows the highest dependency on fossil fuels. Petroleum, diesel and kerosene, burned in internal combustion engines, cover 94% of the energy demand for transport. Accordingly, the share of liquid and gaseous biofuels (8 PJ, 3%) is currently very low, also because Switzerland did not mandate a biofuel quota as in place in many European countries. Electricity is used to operate trains and to a very small extent (0.2 PJ) battery electric vehicles (Fig. 2b).

Similar to above, the choice of the fuel and the engine depends on the type of vehicle. Currently, slightly less than half of the fuel consumption (149 PJ) is caused by private passenger transport with cars, followed by international air transport with departure in Switzerland (78 PJ, 25%). Freight transport by road is carried

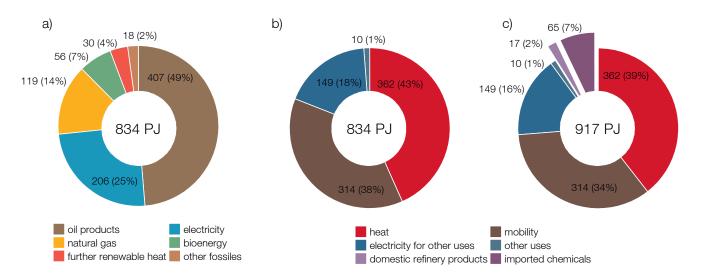


Fig. 1. Final energy demand in Switzerland in 2019. a) Contribution of fossil and renewable energy carriers and sources to the final energy demand including international aviation. b) Final energy demand by purpose. [4] Electricity for other uses than heat and transport includes for example power units, light and communication. c) Final energy demand including the non-energetic use of fossil resources.

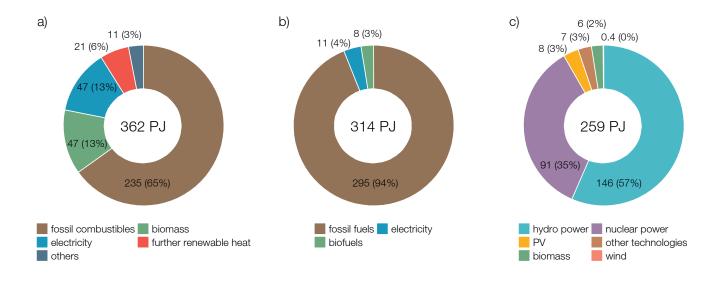


Fig. 2. Energy sources and technologies for the main contributing sectors to the final energy demand in 2019: a) heat supply, b) transport and c) electricity. For electricity, the actual production including the export part and the fraction that is used for storage pumps is shown, which is thus higher than the final electricity demand.

out by trucks and delivery vans and contributes 14% to the energy consumption, while total rail transport accounts for only 3%.

2.3 Current Technologies and Energy Sources for Electricity Supply

The current annual final electricity demand amounts to 206 PJ, whereas 149 PJ are used for other purposes than heat and transport. In contrast to the other sectors, the share of renewable energy in the Swiss electricity mix is already comparably high mainly due to the large capacity of the hydropower plants (146 PJ, 57%) (Fig. 2c). Minor shares of renewable electricity are contributed by photovoltaic panels (8 PJ), by biomass-based power plants (7 PJ) and by wind energy (0.4 PJ). Fossil energy sources used for electricity generation include nuclear power (91 PJ, 35%) and natural gas (3%). In contrast to *e.g.* Germany or China, coal is not used in Swiss power plants – although part of the imported electricity is produced from coal.

3. Technologies for a Renewable Energy Sector

For a complete carbon-neutral society, the above-described energy services must be provided completely by renewable technologies or, if this is not possible, the remaining emissions must be mitigated by CCS. Below, we give a short overview about the principal technologies that are available for the different services, together with an estimation of the potential in Switzerland.

3.1 Renewable Heat Supply

Most technologies for renewable heat supply are already in use today, albeit on a small scale. One option is the extended use of biogenic solid or gaseous combustibles in furnaces or CHP plants, respectively. The direct use of biomass as combustible requires a low water content, thus air-dry woody biomass is well suited. However, domestic wood is a scarce resource with an annual sustainable potential of 49 PJ of primary energy. [5] Thus, wood combustion can contribute maximal 42 PJ of heat (calculated with an efficiency of 85%) corresponding to 12% of the current heat demand. Direct burning of wet biomass fractions such as manure is not feasible, however they could be converted by anaerobic digestion or hydrothermal gasification to biogas (see section 6.2), which is then burned. Manure and sewage sludge have a sustain-

able potential of 27 and 5 PJ primary energy after conversion to biogas, respectively. [5] Instead of burning native biomass, it is also possible to use only those fractions of a certain biomass that are difficult to convert to other target products. An example of this is the combustion of lignin after the carbohydrate fraction of the biomass has been converted into bioethanol, thereby generating the necessary process energy and a surplus of electricity. [6] Generally, biogenic combustibles have the advantage that they can generate high-temperature heat, which is required for process heat or to operate a thermal power plant.

Other options for renewable heat production can be summarized under the term 'power to heat', which include heat pumps and electric boilers and furnaces. Heat pumps enable the use of environmental heat (e.g. from below ground, or from water reservoirs) by extracting and elevating it to a higher, useable temperature level. Heat pumps have the advantage of a high efficiency, as with one unit of electrical energy, 2–4 units of thermal energy can be extracted additionally, i.e. the electric efficiency amounts to up to 500%. A heat pump is a confirmed technology to generate heat suitable for space heating (T = 30 to 35 °C), while industrial heat pumps (with working temperatures around 120 °C) are just beginning to be established. For higher temperatures, electric boilers and direct heating systems can be used. These have an electric efficiency of almost 100%. For medium-temperature heat (100-600 °C), the equipment is already on the market and used on some industrial sites. For high-temperature heat (>600 °C), electric furnaces are technologically feasible but not yet as mature.^[7] Currently, for example BASF, SABIC and Linde together are developing an industrial scale electric steamcracker operating at 850 °C,[8] which underpins the potential significance of such equipment. Electric boilers are also increasingly employed for district heating as a method to balance surplus electricity in the grid. However, this requires that the electricity surplus and the heat demand occur within a relatively short period of time, since otherwise large well isolated reservoirs would be needed for the seasonal storage of hot water. For a good environmental performance of heat pumps and especially other electric heating systems, it is essential that renewable electricity is used, as the otherwise occurring conversion chain combustible to power to heat is less efficient than the direct combustion.

Solar thermal collectors use solar radiation to directly heat water or another fluid and are typically used for the generation of warm water. Due to seasonal fluctuations of the heat generation, these systems are mainly used to complement combustible-based heating systems. To avoid competition with photovoltaic panels for space on suitable roofs, hybrid solar collectors producing power and heat could be used.

3.2 Renewable Energy for Transport

For CO₂-neutral mobility, the two principal options are the switch to electric engines, which requires restructuring the current vehicle fleet and transport infrastructure or the use of renewable drop-in liquid fuels which diminishes changes on the demand side. Electric vehicles can be powered by batteries or by fuel cells. Battery electric vehicles of many different manufactures have reached series-production readiness, and the passenger car registrations in Switzerland are increasing from year to year. Generally, electric motors are characterized by an excellent efficiency, being almost a factor of 3 to 4 higher than that of combustion engines.^[9] A disadvantage of batteries is currently the relatively low energy density, which makes them unsuitable for aviation, shipping and potentially less attractive for long-haul heavy-duty trucks. However, in Europe the legally required breaks for the truck driver could be used for recharging and thus battery electric trucks are increasingly regarded as suitable by manufacturers (e.g. Mercedes-Benz, MAN, Volvo, etc.). Alternatively, the integration of a fuel cell generating electricity for the engine from e.g. H₂, methanol or NH₂ is an alternative. The achievable ranges with such vehicles are higher than with the sole battery use, e.g. the US company Nicola claims a range of 1,500 km with its H₂- fueled truck. Furthermore, refilling the tank is much faster than recharging the battery. As renewable H_2 is thought to be synthesized mainly by electrolysis of water, it belongs to the 'power to X (PtX)' fuels and is termed PtH₂.

Alternatively, so-called renewable 'drop-in fuels' are suitable to operate conventional engines without technical adaptations and allow a rapid and seamless integration into today's supply network. As internal combustion engines are less efficient than electric engines, drop-in fuels are especially relevant for applications that do not allow for direct electrification, such as aviation or shipping. Examples for these drop-in fuels include biodiesel, which consists of long-chain fatty acids derived from plant oils or animal fats esterified with methanol, or HEFA (hydroprocessed esters and fatty acids) fuels, which are produced by hydrogenating vegetable oils or animal fats and can be used both as biodiesel and as biokerosene. However, the costs, the limited availability and the often non-sustainable production of the feedstocks are major challenges that likely do not allow a large expansion of the technology.[10] Additionally, liquid drop-in fuels can be synthesized from CO₂ and H₂ (see section 6.3) and are termed 'Power to liquid (PtL)'.

For a first evaluation of the different electricity-based propulsion technologies (*i.e.* electric vehicles or PtX fueled internal combustion engines vehicles), a relatively straightforward calculation of the corresponding total energy efficiencies (electric energy input vs. propulsion energy output) is helpful. Ueckerdt *et al.* ^[9] calculated an efficiency of 81% for battery electric cars, compared to an efficiency of only 16% for a PtL fueled conventional car (Fig. 3a, d). Thus, the electricity demand per kilometer driven is five times higher for a PtL fueled vehicle compared to a battery electric vehicle.

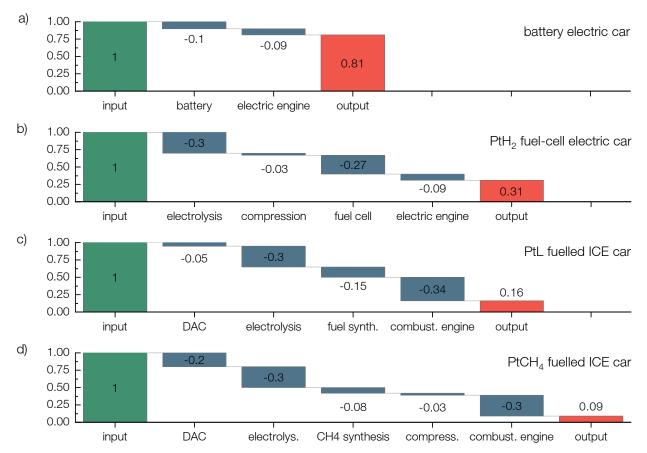


Fig. 3. Energy losses in the steps from fuel production to propulsion. a) Battery electric car, [9] b) Power to H₂ fuel-cell electric car, [11] c) PtL fueled internal combustion engine car, [11] (The difference in energy consumption for DAC is due to different assumptions in the studies.)

A study by Sutter *et al*.^[11] calculated an even lower efficiency of 9% for a power to CH₄ (PtCH₄) fueled internal combustion engine car, but stated an efficiency of 31% for a PtH₂ fuel cell car, which reduces the efficiency penalty of the PtX fuel to a value just over two. Based on these calculations, it can be concluded that PtX fuels are a valuable option for difficult to defossilize sectors and applications such as long-distance aviation or shipping, but currently not for light duty vehicles that can be electrified directly.

3.3 Renewable Electricity Supply

As evident from the previous sections, renewable electricity supply is key for the transition to a low carbon society. Similar to the situation in the heat sector, the technologies to reach this goal are already well advanced and available today, but their use has to be expanded. Hydropower and wind power have a relatively low additional potential in Switzerland of 12^[12] and 32 PJ,^[13] respectively. In contrast, photovoltaics have a much higher technical potential, which is estimated at 86 to 240 PJ.[14] However, the short-term fluctuating supply of especially wind and solar electricity (and to a lesser extent of longer-term fluctuations of run-of-river power plants) is a major challenge for the electricity grid. It is estimated that for every 11-18 PJ/a of solar power production, about 1 GW of control power is needed to match power supply and power demand. Therefore, new electricity control and storage technologies must be developed to stabilize the grids. The most frequently discussed control mechanism is the evolution from traditional power grids to smart grids enabling a two-way flow of electricity and data with digital communications technology allowing to match electricity consumption and production. Additionally, possibilities to store electricity in a suitable form are needed, both on a short-term (to buffer daily fluctuations) as well as on long-term time scale (to buffer seasonal fluctuations). Possible storage technologies are e.g. batteries, pumped storage power stations and PtCH₄ or PtH₂ with storage in the natural gas grid or tanks, respectively.[2] Biomass can also be used to compensate for both short-term and seasonal fluctuations. For example, biogas can be combusted on demand in CHP plants to balance short-term load fluctuations, since the involved engines have very short reaction times. Additionally, solid biomass-based power plants could be used only in times when the supply with e.g. photovoltaic electricity is low in the winter months to balance seasonal fluctuations. Such types of power plants would produce additional band load, as they cannot be switched on or off quickly. However, the provision of power plants that are only used parttime will increase the cost of electricity.

3.4 Carbon Capture and Storage

There is broad consensus that CCS and negative emissions technologies (NET) will need to be employed to reach the climate goals, as some GHG emissions, *e.g.* CO₂ from cement plants or nitrous gases from agricultural activities, are impossible or at least very difficult to avoid. If carbon is captured from fossil point sources such as a power plant, CCS enables the CO₂ neutral use of fossil carbon. However, if the carbon is captured from the atmosphere, or if biogenic carbon is captured, *e.g.* from a bioenergy plant – a combination termed 'bioenergy with carbon capture and storage' (BECCS), negative emissions are achieved, *i.e.* CO₂ is removed from the atmosphere. [15]

The first process in the value chain for CCS is the biological (as done by plants) or technical capture of CO_2 . Technical capture is most economic from point sources, where high concentrations of CO_2 are released, *e.g.* from power plants, but also from cement production or fermentation facilities and a suite of technologies is available or under development. For power plants, post- and oxycombustion CO_2 capture are the main process configurations. [16] In post-combustion capture, a fuel is burned with air and CO_2 is captured from the flue gas after power generation. This configura-

tion requires the separation of N_2 and CO_2 , which is possible by selective absorption of CO_2 for example in concentrated aqueous amine solutions. Stripping with water vapor at elevated temperatures allows the release of CO_2 from the absorbent. Pressure swing adsorption of CO_2 , for example on activated carbon or zeolites, is another attractive technology, which potentially has a lower environmental footprint in comparison to amine absorption, however, it is less mature. [17] Post-combustion CO_2 capture can be retrofitted to existing plants and several large-scale demonstration projects are in operation capturing up to 8.4 million tons of CO_2 per year, with the majority being located in the United States. [18] In oxy-combustion CO_2 capture, pure oxygen derived by air separation through cryogenic distillation is used to combust the fuel. In this case, the flue gas consists only of CO_2 and water vapor, which can straightforwardly be separated in a condenser.

In addition to point source capture (PSC), CO₂ can also be removed directly from the atmosphere, which is termed 'direct air capture' (DAC). The atmospheric CO₂ concentration is with 0.04% by a factor of 100 to 300 times smaller than in the flue gas of power plants, thus huge volumes of gas need to be processed. Assuming a 50% CO₂ recovery, around 2,500 m³ air must be treated to capture 1 kg of CO₂. [18] Technologies for DAC require a high affinity for CO₂, as exhibited for example by aqueous hydroxide solutions or by adsorbents functionalized with alkali carbonates or amines. DAC is commercialized in Switzerland by the company Climeworks, who operates a small demonstration plant in Hinwil with an annual isolation of 900 t of CO₂ and is constructing a 4,000 tons per year plant in Iceland.

After capturing and release, transport of CO₂ – usually in the supercritical state – to the final disposal site can occur through pipelines, but also with ships, trains, or trucks, especially for smaller first of its kind demonstration CCS projects. For storage, CO, is injected into underground geological reservoirs of porous rocks at a depth of a least 800 m, such as saline aquifer formations or depleted oil or gas fields either on-shore or off-shore, overlaid by an impermeable layer of rocks preventing the escape of CO2. [16] Such CO2 injections have been practiced since many decades in the US as they enable the recovery of additional oil from reservoirs whose extraction by primary methods has ceased - a technology known as enhanced oil recovery (EOR). In EOR, part of the CO, remains underground and additional CO₂ can be permanently stored with relatively little effort and costs by re-injection of recycled CO₂. The additional revenues from the recovered oil decrease the costs of CO₂ storage. In Europe, Norway has a pioneering role in exploring CCS. It hosts the world's first and longest running commercial CCS project that started in 1996 and has up to now sequestered more than 20 Mt of CO₂ in the Sleipner gas field located in the North Sea. Furthermore, Norway announced plans to offer its CCS sites to other European countries. The potential for CO₂ storage in Switzerland was so far only theoretically estimated to approximately 2,700 Mt.[19] An alternative to geological storage is soil carbon sequestration, which comprises the application of a non-degradable biochar on agricultural fields as well as the adaptation of agricultural practices in a manner that limits aerobic microbial decomposition of the plant residues.

4. Scenarios for a Net-zero Emissions Energy System

As apparent from the above description of technologies, there is quite a choice of technologies to replace the current fossil services and products. To propose scenarios for a future energy system of a specific country based on these technologies, whole-energy system models are programmed [20] that generate solutions fitting to the chosen optimization parameters (e.g. minimal costs, maximal CO_2 savings) and available constraints (e.g. potential, maximal allowed costs). Below, recent scenarios for Switzerland and a global scenario are presented.

4.1 Scenarios for a Net-zero Emissions System in Switzerland

For Switzerland, the study 'Energieperspektiven 2050+', which was mandated by the Swiss Federal Office of Energy, presents and evaluates possible scenarios to a climate neutral society in 2050.^[2] In the following, we only describe the basic scenario entitled 'zero'. Overall, the total final energy demand (with international aviation) is expected to decrease to 584 PJ in 2050, which is approximately 30% lower than the current demand. The dominant energy sources for this will be renewable electricity (228 PJ, 40%), renewable heat (133 PJ, 23%), PtX (115 PJ, 20%) and biomass (88 PJ, 15%) (Fig. 4a). Fossil resources including oil, natural gas and non-biogenic waste contribute 21 PJ and the corresponding CO₂ emissions will be captured and stored.

The demand for heat is with 266 PJ in 2050 still the largest driver of the final energy demand (Fig. 4b). Fig. 5a shows the anticipated technologies and primary energy sources for this purpose. Heat pumps will become the most important heating system, with a corresponding increase from around 0.3 million units today to 1.5 million in 2050. They contribute with 90 PJ of environmen-

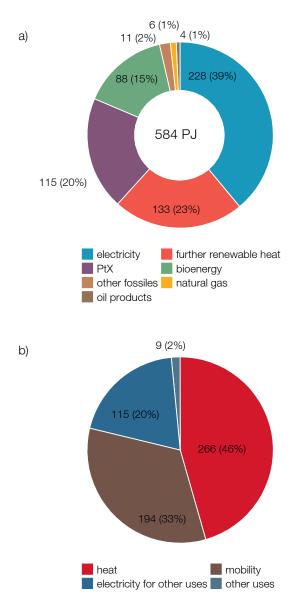


Fig. 4. Projected final energy demand in Switzerland in 2050. a) Contribution of fossil and renewable energy carriers and sources to the final energy demand including international aviation. b) Final energy demand by purpose.

tal heat the biggest share to the category 'further renewable heat' (110 PJ, 41%) together with 40 PJ of heat produced directly from the electricity required for the heat pumps. Combustion of biomass yields 68 PJ (26%) of heat, while 22 PJ of electricity are used in other electric heating systems. Only a very small share of the final heat demand (12 PJ, 5%) is covered by the fossil resources oil, natural gas, and non-biogenic waste.

The total energy demand for transport will be with 194 PJ in 2050 around 40% lower than in 2019, which can be explained by the wide employment of highly efficient battery electric cars for individual transport. As aviation (64 PJ) and partly also heavyduty trucks will continue to rely on internal combustion engines, but running in 2050 mainly with imported PtL fuels, these will contribute with 100 PJ the largest share of the final energy demand for transport. Together with 15 PJ of PtH₂ produced domestically by electrolysis in run-of-river power stations and used for fuel cell cars, a total of 115 PJ of PtX fuels will be used. Electric vehicles will consume 61 PJ of electricity stored in batteries and liquid and gaseous biofuels will cover 18 PJ of the final energy demand for transport (Fig. 5b).

The total final electricity demand increases until 2050 by 11% to 228 PJ. The total electricity production (316 PJ) is larger than the final demand due to losses and self-consumption of the equipment. In 2050, the two main pillars of the power mix are hydropower (161 PJ, 51%) and photovoltaic plants (121 PJ, 38%). Wind energy (15 PJ), geothermal energy (7 PJ) and bioenergy (8 PJ) are the further renewable technologies complementing electricity generation, while only 6 PJ of electricity are generated from fossil resources (Fig. 5c). It is worth noting that the import of 100 PJ PtL fuels corresponds to an indirect electricity import of 289 PJ (calculated with an energy efficiency of $0.53^{[9]}$), *i.e.* domestic production of these fuels would require the electricity production to almost double.

Overall, these measures decrease greenhouse gas emissions from 46 Mt in 2019 to 12 Mt CO₂ equivalents, which are derived from agricultural activities, certain industries such as the cement and the chemical industry as well as by burning fossil waste. Thus, the large point emitters will be equipped with carbon capture facilities and connected to storage facilities and a bit more than a quarter of the 2019 emissions will need to be sequestrated.

A study by Li *et al*.^[21] also elucidated whether it is feasible to reach GHG neutrality in Switzerland, whereas the authors focused on carbon flows in the system and details on the energy flows were not revealed. In agreement with the 'Energieperspektiven 2050+', the study suggested that net-zero emissions until 2050 can be reached, however necessitates the capture of as much as 20 Mt of CO₂, of which 14 Mt or 30% of today's emissions will be sequestrated.

4.2 Global Roadmap

Recently, the International Energy Agency (IEA) published a global roadmap on how to reach a net-zero emissions world by 2050, abbreviated with NZE.[22] It is based on seven key principles: energy efficiency, behavioral changes, electrification, renewables, hydrogen and hydrogen-based fuels, bioenergy, and CCS. Overall, the total global energy demand declines by 20% from 2019 to 2050 and will amount to 344 EJ (i.e. $344 \cdot 10^{18} \text{ J}$). Electricity covers almost half of the total final energy demand, followed by remaining fossil fuels (21%), bioenergy (14%) and PtX fuels (10%) (Fig. 6a). Two-thirds of the total electricity are generated by wind power and photovoltaics, followed by hydro power (Fig. 6b). Interestingly, the roadmap states that a net-zero system will not be possible without nuclear power, the use of which is predicted to even increase by 2050. In the NZE about a fifth of the global CO₂ emission in 2019 will be mitigated by CCS to reach carbon-neutrality.

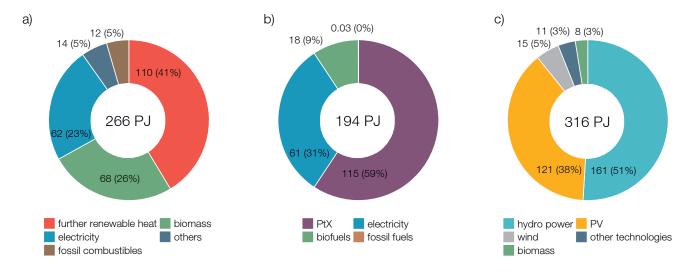
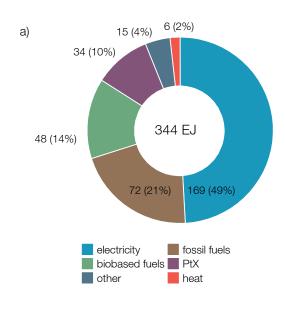


Fig. 5. Energy sources and technologies for the main contributing sectors to the final energy demand in 2050. a) heat supply, b) transport and c) electricity.

5. Current Demand of Fossil Resources for Nonenergetic Purposes

Fossil resources are not only used to provide energy, but they currently also serve as the prime feedstock for the conversion to chemicals. For example, the feedstock mixture of the German chemical industry consisted in 2017 of 75% naphtha – an oil refining product – and other oil derivatives, 11% natural gas, 1% coal and 13% biomass.[23] The renewable production of chemicals is often a blind spot in the discussion of the energy turnaround, but this contribution is quite relevant. Globally, approximately 14% of the total oil consumption and 8% of consumed natural gas is used to produce chemicals, whereas just over half of this is used as feedstock.^[24] Currently, the chemistry sector with its enormous product diversity is largely based on only seven primary chemicals. The production of these seven primary chemicals accounts for approximately two-thirds of the sector's total fossil resources consumption.^[24] Ammonia is synthesized by the Haber-Bosch process from N₂ and H₂. Hydrogen for this process is typically produced by steam reforming of natural gas to syngas – a gaseous mixture of mainly CO and H₂ – followed by the water gas shift reaction (CO + $H_2O \rightleftharpoons H_2 + \dot{C}O_2$). Overall, the process intrinsic CO₂ emission amounts to 1.3 t CO₂ per t of NH₃. [25] For methanol production, again steam reforming of natural gas is the key process, whereas here the syngas is further converted to methanol. The other five primary chemicals ethylene, propylene, benzene, toluene and mixed xylenes - collectively referred to as high value chemicals (HVC) – are co-produced typically by steam cracking of naphtha. Coal as complementing carbon source for petrochemicals production is relevant especially in emerging countries such as China.

The chemical industry in Switzerland is not engaged in the production of primary chemicals but rather imports plastics and the required chemicals e.g. for synthesis of fine and specialty chemicals. According to data published by the Swiss customs, in 2019 the net-import (i.e. the import minus the export) of chemicals and plastics amounted to 1.6 Mt. Based on the carbon content of the products, we estimated that this corresponds approximately to 1.5 Mt (65 PJ) of oil (see Supplementary Information for details). Furthermore, the Swiss energy statistic reported the consumption of 0.4 Mt of oil (17 PJ) for non-energetic purposes, for example as lubricants for machines and vehicles or as bitumen for road construction. Overall, the non-energetic use of oil in Switzerland amounts to 1.9 Mt, which corresponds to 20% of the total energetic oil consumption (9.5 Mt, 407 PJ) and to 9% of the total final energy demand (Fig. 1c).



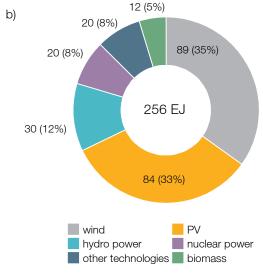


Fig. 6. Global contribution of fossil and renewable energy sources to a) the final energy demand in 2050 and b) to the electricity production. [22]

6. Technologies for the Sustainable Production of Chemicals

All organic chemicals are carbon-containing molecules, which makes a carbon source mandatory for their production. Thus, for the chemical industry, the term 'decarbonization' does not make sense, but rather a 'defossilization' must take place. In principle, biomass, CO₂ and recycled plastics are available as renewable carbon sources for this purpose. [26] Furthermore, H₂ is needed for many reactions, and renewable hydrogen sources are water and biomass. The development of synthetic routes based on these feedstocks is receiving considerable interest, not only from academia, [27,28] but also from industry-related organizations. [29,30] For example, in Germany the Renewable Carbon Initiative was recently founded and has several industrial members including *e.g.* Beiersdorf, Henkel, Givaudan and Firmenich. [26]

In the following, we outline briefly selected important processing routes from renewable resources to H₂ and to today's seven primary chemicals. This direct replacement of fossil products without changes to the established value chain is termed the drop-in strategy^[28] and seems to be favorized according to the industry-backed roadmaps for a cleaner chemical sector (see section 7). Possible routes and products for the 'emerging strategy', where new products and new value chains are created, are presented in section 8.

6.1 Renewable Hydrogen Production

So called 'green' hydrogen can be produced from water or from biomass: Water splitting by electrolysis leads to O₂ and H₂. The achievable efficiency of the conversion from electric energy to hydrogen (lower heating value) is approximately 75%^[25] and the conversion is only carbon neutral if clean electricity is available. Similar to the conventional hydrogen production from natural gas, also biomass can be converted first to syngas, followed by the water gas shift reaction.^[31] If this process is coupled with CCS, it is CO₂ negative. Alternatively, biomass can be converted first to biogas by anaerobic digestion or hydrothermal gasification (see section 6.2), followed by steam reforming. 'Turquoise' hydrogen is produced by methane pyrolysis, a thermo-catalytic process that splits CH₄ directly into its components H₂ and elemental carbon, that can be stored or used in other products.^[29] Obviously, this process is not based on a renewable resource, however, as it reduces CO₂ emissions from hydrogen production, it is regarded as a valuable option.

6.2 Biomass as Renewable Carbon Source

Plant biomass is a highly diverse, heterogeneous renewable carbon source whose composition, characteristics and ease of transformation to valuable products vary considerably. However, for the drop-in strategy, only few important conversion routes of lignocellulose exist.

In the thermochemical gasification route, whole biomass or also unreacted biomass residues such as lignin are subjected to elevated temperatures (850–1,500 °C) in the presence of oxygen, air or steam, to form syngas. Thus, in this step all biomass components are funneled to a homogenous gaseous product mixture analogue to its fossil counterpart. Prior to further processing of the syngas to the target products, it must be purified by a multistep gas cleaning procedure, as it contains numerous impurities that are harmful either to the catalysts used downstream or to the technical components of the plant. Syngas is a versatile intermediate product that can be converted to methane (then termed 'synthetic natural gas'), to methanol or to synthetic naphtha by utilizing the Fischer-Tropsch process. Such biobased naphtha can then be steam-cracked to HVCs. Alternatively, syngas can be used as a substrate for microbial fermentations yielding, for example, ethanol, an approach that is pursued by the New Zealand based company LanzaTech. Dehydration of ethanol yields the HVC ethylene. A further thermochemical conversion method, that in contrast to gasification is suitable for wet biomass streams, is the catalytic hydrothermal gasification to SNG. Here, pretreatment and drying of the biomass can be avoided. Furthermore, inorganic salts, such as phosphorous compounds, can be recovered and used as nutrients.

Ethanol as the starting material for ethylene synthesis can also be produced from the carbohydrate fraction of biomass by biochemical conversion methods. Since lignocellulose has a high recalcitrance towards enzymes and microorganisms, a physicochemical pre-treatment must be carried out to enable a sufficiently fast and high yielding subsequent enzymatic hydrolysis step releasing fermentable, soluble sugars. Microbial fermentation of these sugars with e.g. a yeast strain gives ethanol as final product as demonstrated and marketed for example by Clariant in the SunLiquid process.^[32] Another biochemical conversion route is the anaerobic digestion of manure or other wet biomass types to biogas. Anaerobic digestion is a complex biochemical degradation process performed by a natural, undefined consortium of bacteria and archaea at temperatures of around 37-55 °C. It can be performed in small, decentralized agricultural plants and one of the valuable assets of the process is that the biogas separates spontaneously from the reaction slurry thereby facilitating product capture and purification. By selective removal of CO₂, biogas can be upgraded to pure methane.

Calculations of the IEA showed that around half of the global estimated sustainable potential of biomass (or 68 EJ) would be needed if the primary chemicals were to be produced solely from this resource as carbon and energy source. [24] Also in Switzerland the sustainable available amount of carbon contained in biomass (3 Mt)[33] is higher than the carbon content of the imported chemicals (1 Mt) suggesting that biomass could theoretically cover the feedstock demand for chemicals. However, producing chemicals on a commercial scale from biomass is complex and the technology is by far not as mature as conventional fossilbased chemical plants, which determine current world market prices. Furthermore, biomass is a seasonal product, which means that storage facilities must be set up to guarantee constant availability. Also, harvesting and pooling of biomass is relatively costly because it is spread over large areas and the energy density is low. Therefore, logistics limit the dimensioning of a biorefinery to a modest size compared to today's oil refineries and positive economies of scale, *i.e.* the reduction of production costs for larger plants, can thus only be realized to a limited extent.[34] Biochemical conversions of lignocellulose require a pretreatment step, but this is particularly difficult on an industrial scale as, for example, high sand and dirt contents of up to 25% result in rapid wear of the reactors used. For the gasification processes, gas purification costs are one of the main challenges, and amount to about twice the costs compared to when natural gas is used.[35]

6.3 CO

Although CO₂ is often only regarded as a harmful GHG gas, it can also be employed as a carbon source for organic chemicals after being captured (see section 3.4). For many conversions, hydrogen is necessary as a co-substrate to activate the inert CO₂ molecule and to form the desired PtX product. This strategy is also known as 'carbon capture and utilization (CCU)'. A mixture of CO₂ and H₂ can be converted to syngas by the water gas shift reaction, and subsequent Fischer-Tropsch reactions yield synthetic naphtha.^[29] This in turn opens up the conventional route to HVCs by steam cracking. Direct hydrogenation of CO₂ yields methanol, which can further be converted to HVCs by the methanol-to-olefins and methanol-to-aromatics processes. The Sabatier reaction enables the methanation of CO₂ with H₂ for the production of synthetic natural gas.

Simulations show that CCU has the potential to make global chemical production independent of fossil carbon sources. [36] However, the increased use of CO₂ raises energy consumption – and would result in an additional electricity consumption of up to 55% of today's global electricity production. [24] In addition, considerably larger mass flows of raw materials would have to be processed, as CO₂ has a low carbon content of only 27% w/w.

6.4 Recycled Plastics

Recycled plastics are supplementing biomass and CO₂ as carbon source and lower the feedstock demand for production of new plastics. In mechanical recycling of plastic, the waste is sorted to collect the desired polymer such as *e.g.* PET, shredded, melted and finally transformed into a new product, *e.g.* plastic bottles. The disadvantage of this method is that the quality of the recycled polymer is often lower than that of the original product. Chemical recycling, *i.e.* the molecular deconstruction of the plastic and the subsequent reconstitution, diminishes or completely avoids the issue of reduced quality. Both gasification followed by Fischer-Tropsch synthesis as well as pyrolysis (*i.e.* a thermal decomposition in an inert atmosphere) lead to synthetic naphtha as a source for HVCs for plastic synthesis. ^[29] Alternatively, for some plastics the targeted depolymerization to the monomeric building blocks for example by solvolysis and repolymerization is possible. ^[37]

Calculations by the IEA suggest that a quote of 40% plastic recycling could save up to 70 Mt of primary chemicals, which corresponds to roughly 10% of today's production. Thus, recycling of plastics would help to close material cycles and contribute to a circular economy but will never be a standalone solution to defossilize the chemical industry.^[26]

6.5 Comparison of Fossil, Biomass, or CO₂-based Production of Methanol

Direct comparisons of different renewable production paths with regard to their sustainability are so far seldom reported. For instance, Gabrielli et al.[38] provided a qualitative comparison for different production routes of methanol, that is underpinned by energy demand calculations. Six synthesis routes were analyzed in the framework of a net-zero emissions world. Here, the necessary carbon is derived from i) fossil fuels coupled with CCS (CCS route), ii) captured CO₂ (CCU route) or iii) from biomass (BIO route). Both possibilities for carbon capture, i.e. DAC and PSC, were considered. The CCU routes require the highest amount of energy, around 6 to 7 times more than the BIO route and 2 to 5 times more than the CCS routes, as the H, production consumes a high amount of electric energy (Fig. 7). If the power is not CO₂ free, the CO₂ emissions of the CCU routes grow 8 to 10 times faster with increasing carbon intensity of the electricity than those of the CCS and BIO-routes.

7. Scenarios for a Renewable Chemical Industry

To derive a perception of how a more sustainable chemical industry as a whole could likely be reached, we will summarize in this section two published scenarios, but due to a lack of data not for Switzerland, but for Germany and globally.

A study by DECHEMA investigated possibilities to reach a GHG neutral chemical industry in Germany in 2050.^[29] In contrast to Switzerland, the German chemical industry also produces the primary petrochemicals and the study specifically looked at alternative production processes for these. For methanol and ammonia production, the hydrogen production by electrolysis or methane pyrolysis was considered, while the HVCs are assumed to be produced from biogenic or synthetic naphtha (see section 6 for a brief description of the possible technologies). The calculations of the CO₂ footprint consider the energy demand for the production processes, the process emissions themselves and the carbon content in the chemicals as a source for CO₂ at the end of life

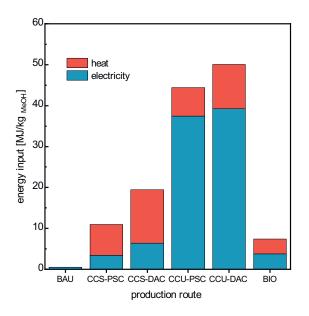


Fig. 7. Power and heat demand for methanol production by different routes. [38] BAU: business as usual; BIO: from biomass; PSC: from point source; DAC: direct-air-capture; CCS: carbon capture and storage; CCU: carbon capture and utilization

stage. Only the currently unused lignocellulosic biomass potential in Germany was assumed to be available for chemical production. CCS was not included as an option to decrease CO_2 emissions. The study defined two paths for improving the sustainability of the chemical industry. The 'technology path' describes possible GHG savings under the prerequisite that new technologies are only introduced if they are economically feasible. Furthermore, an upper limit for power consumption was defined for this path. Under these assumptions, a technology portfolio was suggested that allows GHG emissions to be reduced by 61% compared to 2020, however accompanied with an increase in power demand by a factor of 4. The suggested technology mix and resulting feed-stock mix are depicted in Fig. 8.

A second path termed 'GHG neutrality' was investigated, where all restrictions regarding costs and electricity availability were lifted. With this, a net-zero chemical industry would be possible, which would lead, however, to an increase of the electricity demand of the chemical industry by a factor of 11 relative to the need in 2020 and would require around 3 times higher investments in infrastructure than for the technology path. As the available amounts of biomass and plastic waste would completely be used also in the technology path, the remaining fossil carbon could – under the assumption of no CCS – only be replaced by CO₂, which would become the most important feedstock (Fig. 8).

A study issued by the IEA offers a global view on the future of the petrochemicals sector and proposed a so-called 'clean technology scenario (CTS)' to decrease GHG emissions in this sector by 45% in 2050 compared to 2017. This is already quite ambitious, considering the projected increase in primary chemicals output by 40% driven by the strong increase in global plastic demand. Overall, the CTS is optimized for cost efficiency of the measures and builds on five pillars for GHG emissions reductions, with the corresponding relative contributions given in brackets: CCUS (35%), the transition from coal to natural gas as feedstock (25%), enhanced energy efficiency (25%), plastics recycling (9%) and alternative feedstocks (6%). Oil and natural gas remain the main feedstocks in the CTS for chemicals production while biomass and hydrogen contribute only marginally on the global scale.

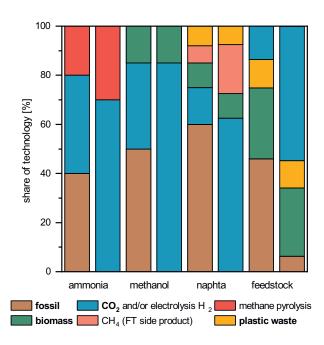


Fig. 8. Suggested technology and feedstock mix for the production of ammonia, methanol and naphtha in the German chemical industry in 2050^[29] according to the technology path (left column of the pair of columns for each product or feedstock) and the GHG neutrality path (right columns).

However, therein Europe is an exemption, as here electrolytic $\rm H_2$ is expected to be used for half of the ammonia and for two-thirds of the methanol production similar to the German GHG-neutrality scenario. Biomass is thought to be fermented to ethanol, followed by dehydration to ethylene, and accounts for less than 5% of the cumulative HVC production. Additionally, an even smaller part of biomass is converted to syngas to produce methanol or hydrogen for ammonia synthesis. Roughly one third (400 Mt) of the $\rm CO_2$ generated by the petrochemicals sector will be captured with around an equal share being used as carbon source for methanol production or being sequestered.

8. The Role of Biomass in the Path to Net-zero GHG Emissions

In the transition to a net-zero GHG emissions energy and feedstock system, biomass has a special role, as it is the most versatile renewable energy and carbon source. It can be used to generate heat and electricity, or it can be converted to biofuels or chemicals to contribute to a renewable transport and chemical sector. Furthermore, biomass can also contribute to CO₂ removal by BECCS. However, the availability of biomass is too limited to serve as the main solution for all these sectors and the optimal use is still debated.^[39] In the following, we first compare the foreseen uses of biomass in the above discussed net-zero pathways. Then, the concept of resource efficiency is introduced by presenting a case study comparing the use of biomass as combustible or as feedstock for chemicals. Finally, we offer a broader view on the potential use of biomass as substrate for further chemicals than only the prime petrochemicals.

8.1 Role of Biomass in Net-zero Scenarios

In the above-described scenarios for a net-zero GHG emission system, the proposed contributions of biomass to the different sectors are quite different from each other. According to the 'Energieperspektiven 2050+', the total energetic use of biomass amounts to 131 PJ, which is covered by the complete use of the sustainable domestic biomass potential (75 PJ) and biomass imports (56 PJ) mainly in the form of biogas. 62 PJ (47%) of the

biomass will be used for heat production, with an approximately equal share between process and space heat. 49 PJ (37%) of biomass is lost for energy transformations, *i.e.* is not counted in the final energy demand as it is used during the conversion to the energy carriers ultimately consumed. For the transport sector, 19 PJ (15%) of the biomass will be used in the form of biofuels and biogas which is a strong increase compared to today.

In the work by *Li et al.*^[21] on the feasibility of net-zero emissions in Switzerland, the focus was on the carbon flows in the system and the corresponding technologies. Thus, it cannot be compared directly to the Energieperspektiven 2050+, but nevertheless gives an interesting perspective on the recommended use of biomass. In the scenario that included a ban of fossil fuels, woody biomass is burned in industrial cogeneration plants (22%w/w of total biomass carbon) to provide heat and power or converted *via* the syngas platform to hydrogen (30%). Non-woody biomass is converted to jet fuels *via* ethanol produced by fermentation as intermediate product (16%) and to synthetic natural gas by hydrothermal gasification (32%).

According to the IEA roadmap,^[22] globally biomass will contribute slightly over 100 EJ or around one fifth of the gross energy supply. The consumption (*i.e.* loss) for transformation operations to *e.g.* biofuels or electricity is the largest contribution (38%), followed by the industry sector (24%), which includes the use of biomass as energy source for process heat and as feedstock (but separate numbers are not published). Liquid and gaseous biofuels for transport have a share of 18% of the total biomass demand, followed by electricity (12%) and as combustible for domestic heat production (9%).

8.2 Resource Efficient Use of Biomass

One way to propose sensible uses of biomass is to take an environmental point of view. For Switzerland, a life cycle assessment study by Vadenbo et al.[40] recommended the complete energetic use of the currently unused biomass fractions, as this is beneficial for the environment according to all indicators considered, excluding only biomass that is also suitable as animal feed. Determining the most resource efficient way to use wood was the aim by a case study at EPF Lausanne conducted in the framework of the NFP 66 - Resource wood. The resource efficiency indicates how much fossil CO₂ emissions can be avoided per unit of carbon in the biomass. Here, a biorefinery was considered that produced butanol, acetone and ethanol via the sugar platform and syngas from the residues. The syngas is used in a combined cycle power plant and provides heat and electricity for the biorefinery. For each unit of biogenic carbon, 0.85 units of fossil carbon are replaced in this model biorefinery. This balance can be compared to the direct combustion of wood for heat production. Under the assumption that a wood boiler replaces a natural gas boiler, only 0.65 units of fossil carbon are replaced per unit of biogenic carbon. The assumed model biorefinery thus replaces 30% more fossil carbon than the corresponding combustion. If it is additionally assumed that the electricity produced in the biorefinery is used to replace heat, that would otherwise have been provided by a boiler fueled with natural gas, by a heat pump (COP of 4), even 2.4 times more fossil CO₂ could be replaced than with the wood used in a boiler.^[34]

8.3 Biomass as Feedstock for Fine Chemicals

The use of biomass as renewable carbon source for the direct replacement of fossil primary chemicals (*i.e.* the drop-in route) was regarded as beneficial in the DECHEMA study, [29] however, biomass might be even better suited to replace other commodity chemicals. Biomass and oil are chemically very different mixtures of molecules. While oil contains mainly C- and H-atoms, biomass also contains a substantial amount of oxygen, *e.g.* carbohydrates contain a bit more than 50%w/w of oxygen and lignin still around 30%. Thus, the overall degree of oxidation in biomass is higher

than in oil.^[28] If the final target product also has a high degree of oxidation, for example as in acetone or acetic acid, the production from biomass via the drop-in route would lead to several changes of the degree of oxidation, which is not very efficient. Furthermore, the available functionality of the feedstock (e.g. aromatic structures) should be utilized, if possible. Thus, promising direct alternative routes from biomass to functionalized molecules should be considered as well and might also pay off economically. An analysis by Straathoff et al.[41] suggested that production of a target molecule from carbohydrates can be competitive, if the production from oil requires more steps and more oxidation reactions, as is the case for e.g. adipic acid, acrylates, and diols. There are indeed several examples, where chemicals are produced from biomass on demonstration scale^[42,43] including lactic acid, succinic acid or butanol, albeit at the current stage from first-generation feedstocks like sugar or starch instead of lignocellulose.

Generally, in analogy to oil refineries, biomass is thought to be processed in biorefineries, where it is converted into a range of biobased products (food, animal feed, chemicals and fabrics) and bioenergy (biofuels, electricity and/or heat) in a sustainable manner and with the fullest possible utilization of all feedstock components. The multi-step conversions in a biorefinery typically proceed through a few intermediate products called 'platforms' from which the product range is developed. To maintain the inherent functionalities of biomass, biotechnological and catalytic conversion methods based on the sugar and lignin platforms are best suited. Ethanol, as described above, is produced via the sugar platform. However, by employing other microorganisms, the sugars could also be converted to a variety of oxygen-containing products including butyric acid, itaconic acid and 1,3-propanediol.[43] Alternatively, also direct chemical-catalytic conversion methods of sugars are developed, for example in the framework of the NCCR Catalysis, which further expands the product spectrum of the sugar platform.

The lignin platform is closely linked to the sugar platform, as lignin is, besides carbohydrates, the most important fraction in lignocellulose. Lignin is an amorphous, crosslinked polymer consisting of three different phenylpropane units and thus could be a valuable source of aromatic chemicals and materials. Anticipated products include phenolic compounds, hydrocarbons, vanillin and other oxidized compounds as well as resins, composites and polymers.[44] However, depolymerizing lignin has proven to be very challenging, especially after it has undergone condensation reactions as is the case for many common pretreatment methods. One promising example, that belongs to the recent 'lignin-first' approaches that aim to enable the chemical valorization of lignin by preventing condensation, is the aldehyde-assisted fractionation developed in the framework of the SCCER BIOSWEET.[45] This process yields a lignin that can be used for the production of ingredients for cosmetics, plastics or fuels, which is further pursued by the EPFL spin-off Bloom Biorenewables Ltd.. Currently, the majority of lignin is burned to generate steam and electricity as process energy and as additional asset besides the main product.^[6]

9. Summary and Conclusion

Achieving net-zero GHG emissions by 2050 globally and in Switzerland is a challenging endeavor requiring dedicated and enhanced efforts to be initiated quickly, but it is generally regarded as technically feasible. The deep electrification of the transport sector and low temperature heat production enables the decarbonization of these two services contributing a major share to the final energy demand. Renewable electricity can be provided by tapping into solar, wind, hydro, biomass and geothermal energy and its widespread implementation should be urgently pursued as it is a key element of the energy transition. The products of the chemical industry including renewable liquid fuels, *e.g.* for aviation, can be defossilized by using the renewable carbon sources biomass,

recycled plastic waste and CO₂, with the latter requiring considerable amounts of electric energy for the electrolysis of water to produce renewable H₂. Despite these technical possibilities, there will always remain some GHG emissions that have to be abated, thus CCS will be necessary to enable the net-zero goal to be reached.

Supplementary Information

Supplementary information is available on https://www.ingenta-connect.com/content/scs/chimia.

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