Techno-economic metrics of carbon utilisation – Part 1

Technological and economical parameters of carbon utilisation and how these parameters vary widely depending on external and technology-specific variables

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Carbon capture, utilisation, and storage (CCUS) is often confused with carbon storage (CS) rather than carbon utilisation (CU). This misunderstanding is logical since, ultimately, CS is a form of waste disposal while CU refers to the new circular world that emphasises more efficient use of resources. With CU being in general more expensive than CS, some CU technologies need further development, which explains the current focus on storage.

Currently, Yokogawa, a leading provider of industrial automation and test and measurement solutions, is performing a strategic decarbonisation study of the Goi industrial area in the Chiba Prefecture at Tokyo Bay (Yokogawa, 2021). The purpose of this research is to make the industrial area net carbon neutral by 2050, preferably using CU rather than CS.

Figure 1 shows the technological and economic parameters in play for CU. Economically, capital costs and different operational costs will affect project viability. In addition, product market demand and the technical readiness level (TRL) for a given CU technology should be considered.

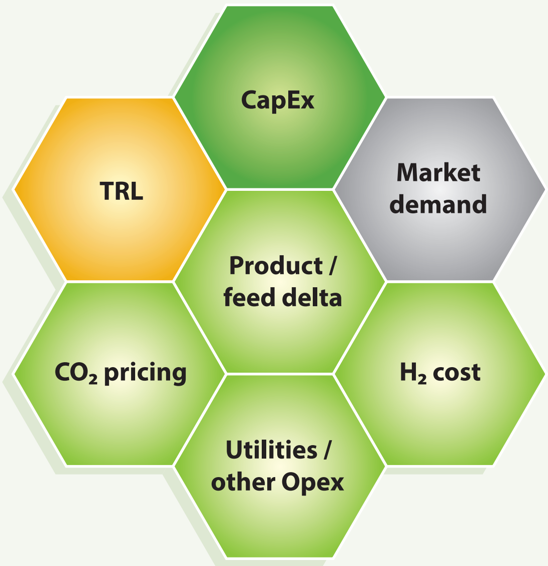

Figure 1 Carbon utilisation: the techno-economic variables

Name	Main products	Non CO_2 feeds	Reaction T (°C)	Capture?
Methanation (Tripodi *et al.*, 2020)	Methane	H_2	200-450	Yes
Methanol (Nyári *et al.*, 2020)	Methanol	H_2	230	No
Fischer-Tropsch (Zang *et al.*, 2021)	Syncrude/SAF	H_2	220-290	Yes
Oxo Synthesis (Liu, 2017)	Butanal	Propylene, H_2	90	Yes
Carbonation (Kamyab *et al.*, 2021)	Building material	Steel slag	35	No
Xylenes (Zhang *et al.*, 2017)	Mixed xylenes	H_2	400	No
Urea (de Haas *et al.*, 2016)	Urea	Ammonia (NH_3)	170	No
Polyols (Fernandez-Dacosta *et al.*, 2017)	Polyether carbonate polyol	Propylene oxide (PO)	135	No
Polymeric Carbonates (Demirel, 2015; Moon *et al.*, 2011)	Polypropylene carbonate (PPC)	Propylene oxide	90	No

Table 1 Carbon utilisation technologies

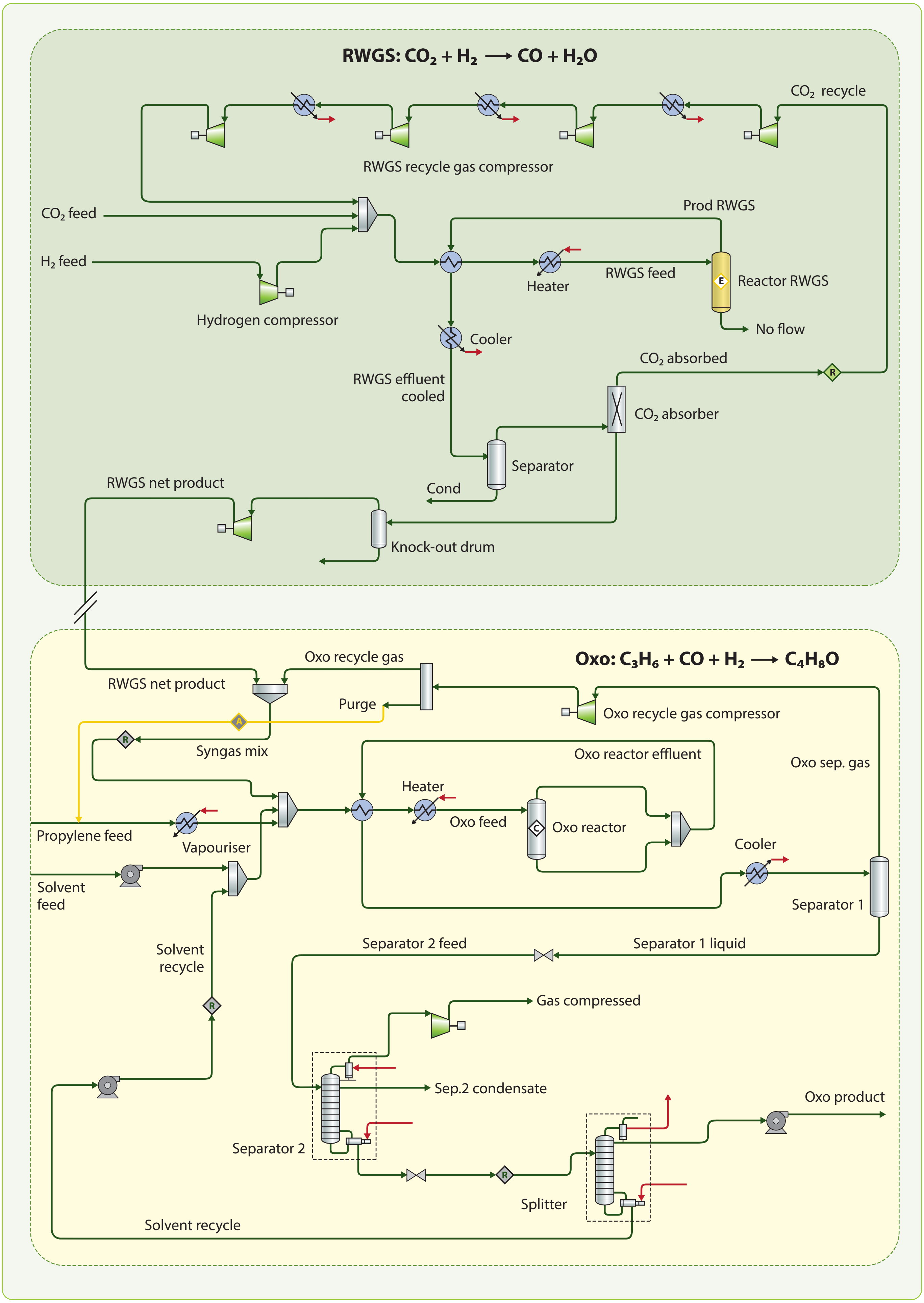

Figure 2 The reverse water gas shift and Oxo synthesis steps of the butanal production process

Carbon utilisation technologies

KBC performed a techno-economic evaluation of the nine CU technologies listed in **Table 1**. **Table 1** also includes the feeds, other than CO_2, and the operating temperature of the CU paths. For most of the feed and product pricing, KBC relied on third-party market intelligence from Argus Media.

The Fischer-Tropsch (FT) and Oxo synthesis configurations considered in the referenced articles consume CO rather than CO_2. Therefore, a reverse water gas shift (RWGS) step is included upstream to convert the CO_2 into CO. The RWGS step includes CO_2 capture to recycle the unconverted CO_2.

The methanation process considered uses CO_2, not syngas (CO). However, due to low CO_2 conversion per reactor pass, a CO_2 capture/recycle step is required, too.

Four of the nine CU technologies were simulated partially or entirely using KBC's Petro-SIM software. **Figure 2** shows the Petro-SIM simulation model of the Oxo process. The technologies were simulated when a process flow diagram was missing, or the assumed process heat integration was incomplete or unrealistic.

Operating cost

Many CU technologies require significant amounts of hydrogen. In the upcoming Part 2 article, we will demonstrate that the hydrogen used for this study should have a very low carbon intensity. The cost of the green hydrogen used and the revenue generated from utilising CO_2 will significantly impact CU technology economics.

Two price scenarios were considered (see **Table 2**). The 2030 scenario employs a high price of green hydrogen and a low price of CO_2. The 2050 scenario adopts a much lower price of green hydrogen and a much higher price of carbon emissions. The price sets correspond with possible carbon and hydrogen pricing in 2030 and 2050. These are semi-arbitrary and based on price scenario trends, not on an in-depth analysis of current and upcoming legislation, carbon markets, and green hydrogen project pipeline. The primary purpose is to demonstrate the sensitivity of the CU economics with carbon and hydrogen pricing.

The 2030 and 2050 price estimates have been established with a more rigorous market analysis by Argus Media for the other feeds (propylene, PO) and the CU products. Yokogawa and KBC established price estimates for the carbonation feeds and PPC products. The estimates are based on price data before third-quarter 2021 inflation rates hit, when natural gas prices wavered around USD 40/MWh rather than surpassing USD 100/MWh.

	2030 Scenario	2050 Scenario
Green hydrogen	USD 4000 /t	USD 1500 /t
CO_2 utilisation revenue	USD 50 /t	USD 200 /t

Table 2 Green hydrogen and CO_2 price scenarios based on pre-inflation 2021 prices

Figures 3 and **4** show the operating cost/revenue breakdown for the different CU technologies under the two H_2/CO_2 pricing scenarios. Hydrogen, other utilities (electricity, fuel, steam), and fixed operating cost are shown on the debit side of the graph, below the zero axis. Revenue streams generated by the product/feed differential and CO_2 utilisation are shown as positive bars in the chart. The resulting operating cost/revenue balance (EBITDA) is plotted in **Figures 5** and **6**.

The charts demonstrate that hydrogen is the key driver of operational costs for many of these technologies. These technologies will only become economically profitable if green hydrogen costs drop significantly, although product pricing can play a decisive role, too. The following sections discuss the operating cost

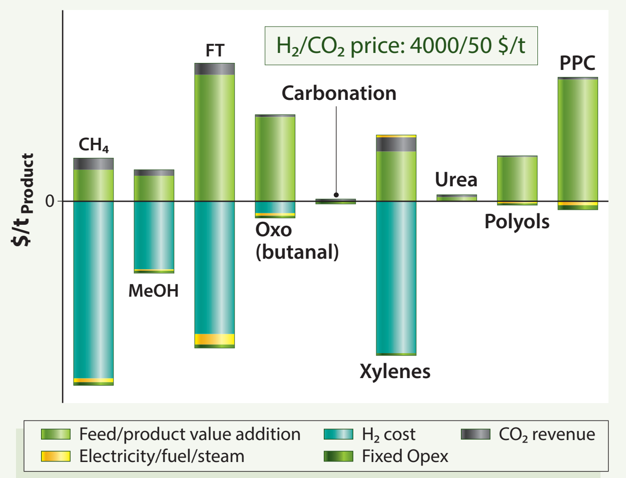

Figure 3 Operating cost/revenue breakdown - 2030 scenario

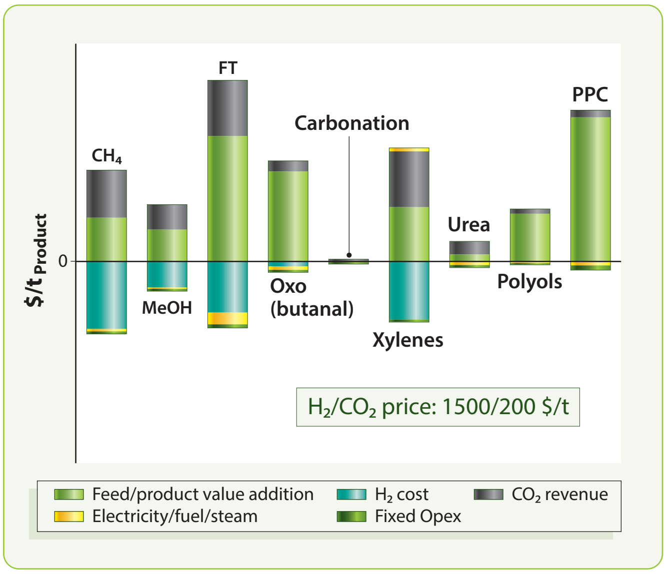

Figure 4 Operating cost/revenue breakdown – 2050 scenario

elements in more detail, as well as the capital cost and technology readiness.

Hydrogen consumed

The hydrogen utilisation intensity (HUI) heavily depends on the CU technology considered and largely correlates with the destination of the oxygen atoms in the utilised CO_2 molecule. The process of producing oxygen-free products involves separating the oxygen atoms in the CO_2 molecule from the carbon atom, which is done by binding the oxygen with hydrogen and generating water. Hence, hydrogen is not only required to generate hydrocarbon but also to capture the oxygen atoms of the CO_2 into water molecules.

The HUI and carbon utilisation intensities (CUI) of the process can be defined as the tonnes of hydrogen and carbon consumed to produce one tonne of product, respectively. **Figure 7** is a theoretical hydrogen intensity chart. The x and y axes are the ratio of the number of oxygen and hydrogen-to-carbon atoms in the product. Acetic acid (CH_3COOH), for example, has an #H/C and #O/C ratio of 2 and 1, respectively. The lines on the graph show lines of equal hydrogen intensity, i.e. lines of equal hydrogen intake for products produced from CO_2, as a function of the oxygen and hydrogen content of the products. Acetic acid is located close to the line of 0.13 $t_{H2}/t_{product}$. Therefore, a green acetic acid facility with a production capacity of 100 t/h of acid out of CO_2 will require just over 13 t/h (~150 kNm^3/h) of hydrogen.

The graph shows that even the production of hydrogen-free carbon from CO_2 requires more than 0.3/t of hydrogen per tonne of product, only to remove the oxygen atoms from CO_2.

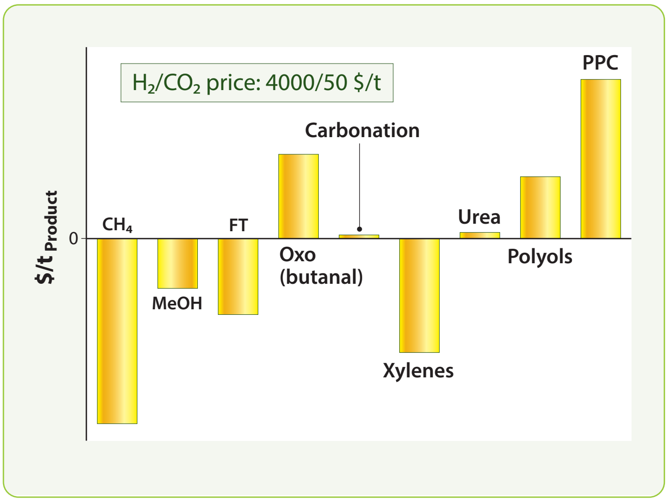

Figure 5 Operating cost/revenue balance – 2030 scenario

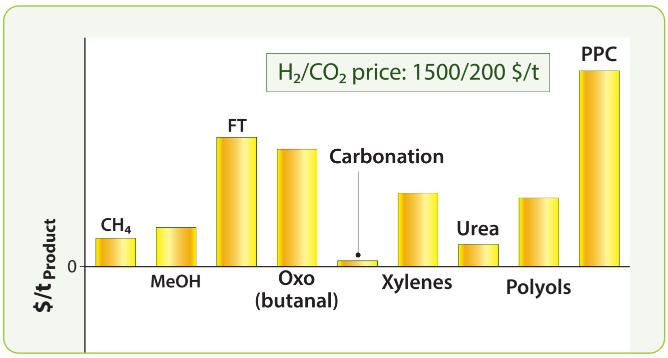

Figure 6 Operating cost/revenue balance – 2050 scenario

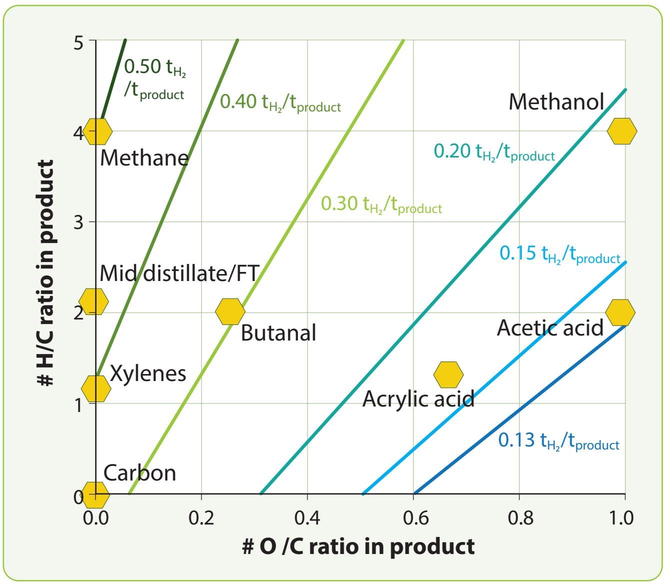

Figure 7 Theoretical H_2 utilisation intensity for product synthesis for CO_2 and H_2

At the same time, the hydrogen requirement drops below 0.2 t/t in most cases if the product contains oxygen.

Producing oxygen-free products from CO_2 requires more hydrogen to remove both oxygen atoms. In addition, removing oxygen from the CO_2 results in products with lower molecular weight, which further increases the H_2 requirement, at least if expressed per tonne of product.

Figure 8 shows the HUI for each of the nine technologies considered. The carbonation, urea, polyol, and PPC technologies require no hydrogen because the CO_2 molecule is bound to another molecule without prior oxygen removal.

Note that the CUI of the FT process tested is close to 0.52 $t_{H2}/t_{Product}$, which is considerably higher than the theoretical intensity of around 0.44 t/t (see **Figure 7**). This is because a significant purge of a syngas stream is applied in the specific process set-up considered in our study (Zang et al., 2021). In **Figure 7**, the hydrogen in that syngas stream has been deducted from gross hydrogen intake, which reaches 0.57 t/t. Even so, the net HUI remains higher than the theoretical value due to the presence of CO in the purge stream. The conversion of CO_2 to CO, which is then purged, requires hydrogen and increases the ratio of hydrogen consumed to FT product produced.

The Oxo synthesis process generates butanal (also known as butyraldehyde, C_4H_8O) from CO_2, hydrogen, and propylene. The use of propylene, which adds hydrogen and carbon to the product, results in the HUI of this process being only a fraction of the theoretical 0.31 $t_{H2}/t_{butanal}$ HUI based on the production of butanal from only H_2 and CO_2. The same applies to the polyol and polypropylene carbonate (PPC) products, which in the technologies investigated use propylene oxide, in addition to hydrogen and CO_2.

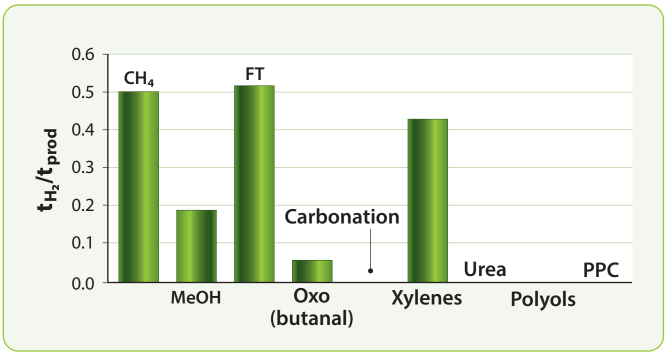

Figure 8 H_2 utilisation intensity for each technology

	2030 Scenario	2050 Scenario
Electricity	0.26	0.00
Fuel/steam	0.14	0.00

Table 3 Electricity and fuel/steam emission factors, tCO_2/MWh

Carbon utilisation: impact on operating revenue

The utilisation of CO_2 is assumed to generate a revenue stream. **Figure 9** shows the CUI for each technology. In general, higher CUIs are preferred.

The CUI data in **Figure 9** includes a correction for the emissions related to electricity and fuel/steam that the process requires or exports. Different electricity and fuel/steam emission factors are assumed for the two cases (see **Table 3**). Therefore, **Figure 9** shows two series of bars. In the 2050 scenario, zero-carbon power and fuel are assumed to be available.

The hydrogen import is assumed to have a zero carbon intensity (CI). If the CI of imported hydrogen is significant, then the CUI of the processes will drop significantly. The utility balance and the impact on the CUI will be discussed in more detail in Part 2.

There is an inverse correlation between CUI and HUI. As mentioned previously, the inclusion of feeds other than CO_2 and hydrogen (oxygen, PO, and propylene) dramatically reduces the relative hydrogen demand. However, it also reduces the CUI.

The carbonation technology, in particular, has

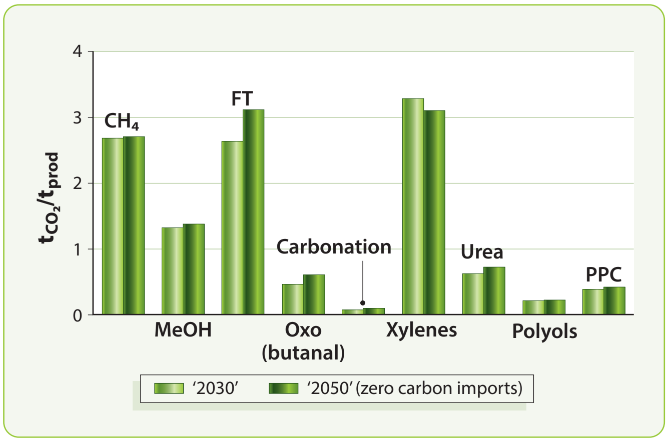

Figure 9 Carbon utilisation intensity of the investigated technologies

a low CUI. Carbonation binds CO_2 to the calcium and magnesium oxide in the slag of the steel plant. The CUI is particularly low because, in addition to calcium oxide (CaO), the slag contains other elements such as silica and alumina.

Product/feed value delta

Natural gas, urea, and methanol are high-volume commodities with a relatively limited product value. The uplift is even smaller for steel slag carbonation. The production of xylenes, polyols, PPC, and butanal offers a slightly to significantly higher product value. The upgrade is tempered in the case of the xylenes technology because nearly half the product mix consists of lower value naphtha or gas.

To forecast product prices, conventional methods such as demand growth and cost-plus-margin approaches were used. Price incentives were not considered for using CO_2 instead of fossil feedstocks due to the current lack of clear legislation, with one exception: sustainable aviation fuel (SAF). Different countries, regions, international institutions, and business organisations are developing legislation and frameworks to facilitate and support SAF production. Similar to renewable diesel in the US, mandates and other support mechanisms are expected to create a new market for high-value products. The SAF price applied in this study is five times higher than fossil mid-distillate products.

SAF represents 40 wt% of the total product mix of the FT technology investigated in this study. With the high SAF price expectations, the value of the combined product mix more than doubles, which has a major impact on the EBITDA, as seen in **Figures 2** to **5**. Indeed, while methane, xylenes, and methanol production all show highly negative cash flows in a high H_2 cost scenario, the FT technology EBITDA is marginally positive, despite the high demand for hydrogen. This difference is wholly due to the SAF price bonus. This SAF price bonus corresponds with a carbon abatement value in the range of USD 500 to 1000/t of CO_2.

Note that all technologies, except for methanation, will be cash flow positive in a high H_2 cost scenario if the CO_2 price reaches USD 350/t. Methanation requires at least USD 700/t.

Road fuels and methane fuel may never benefit from the support SAF is expected to receive because more cost-efficient alternatives are available, i.e. electricity, ammonia, hydrogen, and methanol. Mandates for 'green' chemicals using CU are a potential future low-carbon policy option. Similar to what is currently observed with biodiesel and SAF, this would create a separate market with higher values. These CU-based products are expected to compete with chemicals generated from waste streams.

Fixed operating cost

The fixed operating costs shown in **Figures 3** and **4** include labour, maintenance, insurance, and catalyst/chemicals. The impact of this cost factor is small compared to the other costs.

Some technologies use expensive catalysts that contain noble metals. Similar to naphtha reforming catalysts in conventional oil refining, only a regeneration and lease fee of the noble metal is considered, not the full noble metal value.

In Part 2 of this article, we will dive deeper into the CU technology economics by investigating the capital expenditure for the different technologies and the impact of the CI of green hydrogen, power, and fuel consumption.

Key takeaways

The following can be concluded from the operating cost analysis performed in Part 1:

- Producing fuels and other oxygen-free products requires large amounts of hydrogen, which in the short and medium term makes the technology uneconomical due to the high cost of green hydrogen.
- The potentially very high value of SAF illustrates that production mandates on low-carbon intensity products can change this equation and make CU economically viable at a higher hydrogen cost.
- High-value niche chemicals, especially those containing oxygen, are viable candidates for CU. Producing building materials using CO_2 and slag uses relatively limited amounts of CO_2 but should be economically viable with limited support.

VIEW REFERENCES

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