Process simulation of BECCS-to-X: Investigating the potential of Hydrogen and Sustainable Aviation Fuel Production

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# Abstract

Bioenergy with Carbon Capture and Storage (BECCS) combined with Biomass-to-X (BtX), BECCS-to-X, is a potential technology for generating power and syngas, which can be further processed into useful chemicals and fuels. Herein, the authors discuss and develop process models for converting biomass into hydrogen and sustainable aviation fuel (SAF) – BECCS-to-H2 and BECCS-to-SAF, respectively. Both processes use the same biomass input and produce the same amount of power. Results show the higher energy efficiency for producing H2 (50%) compared to SAF (34%) and total Fischer-Tropsch fuels (47%).

Keywords: BECCS, BECCS-to-X, H2, SAF

# Introduction

Negative Emissions Technologies (NET), such as Bioenergy with Carbon Capture and Storage (BECCS), are essential for achieving Net Zero (DESNZ, 2023). Most scenarios/ pathways to limit global temperature rise to less than 1.5℃ require carbon dioxide removal (CDR) technologies such as BECCS in order to remove CO2 from the atmosphere (Almena, et al., 2022). The generation of useful products from biomass is referred to as Biomass-to-X or BtX (Poluzzi, et al., 2021). BECCS typically refers to thermo-chemical conversion routes with carbon capture and storage (CCS) (Shahbaz, et al., 2021). Thermo-chemical conversion of biomass via gasification produces heat and syngas, downstream processing coupled with power generation can convert biomass resources into both power and useful products, i.e., **BECCS-to-X**.

Depending on the processing route, biomass can be converted into ammonia, bio-char, dimethyl ethers, hydrogen, methane, methanol, and Fischer-Tropsch fuels (Poluzzi, et al., 2021; Hanel, et al., 2022). Hydrogen is an energy carrier and chemical building block, it has the potential to decarbonize industry, power, heating, and transportation (Osman, et al., 2021). Fischer-Tropsch synthesis can produce Sustainable Aviation Fuel (SAF), which is an important mitigation strategy for one of the most difficult to abate industrial sectors - aviation (Doliente, et al., 2020). Hanel et al. (2022) performed an energetic and technical evaluation on gasification based BtX processes. Interestingly, no single optimal BtX was presented, the authors showed the key process indicators (KPIs) are subjective to that processing route. Hence, further investigation for specific scenarios is required.

## Aims & Objectives

This study is a technical evaluation and comparison of BECCS-to-H2 and BECCS-to-SAF using Aspen Plus. The analysis highlights key operating parameters (KOPs) and KPIs for each process. Our previous study focused on the production of H2, whereby hydrogen is separated and purified from bio-syngas alongside CO2 (CCS) with heat-recovery steam generation to provide power (Wilkes, et al., 2023).

The purpose of this paper is to investigate and showcase:

* Process model development and description for BECCS-to-H2 and BECCS-to-SAF.
* Process analysis and identification of KOPs and KPIs.
* Technical comparison between the two BECCS-to-X systems.

# Process description and modelling

The process models are developed in Aspen Plus® v11.1, the model topology for the BECCS-to-H2 and BECCS-to-SAF processes are shown in Figure 1 and Figure 2, respectively. Wet biomass enters and **DRYER** unit and the output moisture content is set to 10.05 wt.%. Within Aspen, biomass is a non-conventional solid and needs to be decomposed (**DECOMP**) into its constituent elements before gasification (**GASI**). An RGibbs reactor is chosen for the gasification unit, which calculates chemical equilibrium based on Gibbs free energy minimization (Tauqir, et al., 2019). The syngas produced in the gasification unit needs upgrading to improve the H2/CO ratio. The syngas upgrading using the water-gas shift (WGS) reaction unit is based on Marcantonio et al. (Marcantonio, et al., 2019) and Moneti et al. (Moneti, et al., 2016), both of which simulated the experiments conducted within the UNIfHY project (UNIfHY, 2016). The WGS reaction (Equation 1) favors the production of CO and H2O at high temperatures, thus the UNIfHY project looked at high temperature shift (HTS) at 400℃ and low temperature shift (LTS) at 200℃. Both **HT-WGS** and **LT-WGS** reactors are operated at 27 bar (Cohce, et al., 2011), and are modelled as REquil reactors representing the WGS reaction (Marcantonio, et al., 2019):

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Sulphur within the biomass is converted into H2S and COS in the gasification unit, and all of the COS is converted in H2S in the WGS units. Therefore, prior to H2/CO2 separation H2S is removed using Selexol, which also co-captures CO2. The separation efficiency for H2S is 100% and for CO2 it is 95% (Chiesa, et al., 2005). H2S is removed in the **SELEXOL1** unit and CO2 is removed in the **SELEXOL2** unit, both are modelled as separation units. The CO2 conditioning unit ensures the CO2 stream is ready for pipeline transportation, it uses sub-critical liquefaction at 66 bar (**CO2-COMP**) and liquid pumping to 111 bar (**CO2-PUMP**) which reduces the energy consumption for the conditioning train (Wilkes, et al., 2021). The energy demand for the Selexol process is 0.6 GJe/tCO2 and 0.63 GJth/tCO2 (Kuramochi, et al., 2012). For the BECCS-to-H2 process, H2 is separated in a pressure swing adsorption (**PSA**) unit (85% capture rate and 99.99% purity (Chiesa, et al., 2005). Heat is recovered in the **HRSG** unit, and the high-pressure steam produces power in the **HP-ST**, **IP-ST**, and **LP-ST** turbines.

BECCS-to-SAF requires additional processing units to convert the syngas into useful Fischer-Tropsch (FT) fuels. The FT reactor model is based on the conversion-based reactor model presented in (Dahl, 2020), using an RStoic reactor in Aspen Plus with conversion data from (Shafer, et al., 2019). The **FT-C** unit is operated at 220℃ and 27.6 bar (Shafer, et al., 2019). Only Paraffins (alkanes) are considered in this study, the overall reaction is shown in Equation 2 (Hillestad, 2015).

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Where is the hydrogen stoichiometric coefficient, is the hydrocarbon stoichiometric coefficient, and the superscript denotes the paraffin component. The heavy hydrocarbons are lumped into . The ASF distribution underestimates the production, thus Equation 3 is added to the RStoic unit.

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The stoichiometric coefficients (Equation 4 and 5) follow the ASF distribution (Hillestad, 2015), where the chain growth factor () is set to 0.9 (Swanson, et al., 2010; Campanario & Ortiz, 2017). The subscript denotes the carbon number. The fractional conversion for the paraffin and methanation reactions is set to 0.394 and 0.077 (Dahl, 2020).

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| Figure 1: Biomass gasification for H2 and power production, model topology using Aspen Plus |

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| Figure 2: Biomass gasification for SAF and power production, model topology using Aspen Plus |

The products from the FT unit are sent to a separation unit (**SEP1**) to separate gaseous hydrocarbons (C1-4), liquid hydrocarbons (C5-21+), and water. Unreacted syngas and gaseous hydrocarbons are recycled. The liquid hydrocarbons are fractionally distillation (**DIST1**) at atmospheric pressure, modelled as a distillation column, to produce commercial hydrocarbon products: gasoline fraction (C5-7), jet fuel fraction (C8-16), diesel fraction (C17-20), and heavy hydrocarbons/waxes (C21+). The heavy hydrocarbons are sent to the hydrocracking unit (**HCRACK**), modelled using an RStoic reactor, which converts the waxes into 50% jet fuel, 30% diesel, 15% gasoline, and 5% light gases. The hydrocracker is operated at 50 bar and 277℃. The process also uses 1.5% H2 sent from the **PSA** unit stationed after the syngas cleaning section and prior to the FT-C. The additional H2 specification ensures the production of middle distillates (mild hydrocracking) (Michaga, et al., 2022).

As the purpose of these processes is to produce H2 and SAF, the hydrogen energy efficiency () and jet fuel energy () efficiency are defined as:

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Where is the mass flowrate in kg/s and the lower heating value (LHV) is in MJ/kg. For the BECCS-to-SAF process there are several useful products that also need to be considered, thus the overall fuel energy () efficiency is defined as (Michaga, et al., 2022):

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The net efficiency in both cases is the electrical efficiency combined with the thermal energy efficiency of the specified fuel type. In the case of BECCS-to-SAF there are two net efficiencies, one for the overall fuel production and one purely for the SAF production.

# Results and discussion

Both models have the same biomass feedstock - hardwood chips proximate and ultimate analysis from (Tauqir, et al., 2019). Both systems process 3,600 kg/hr of biomass with an input energy of 18,850 kW. The air flowrate for the gasification chamber is 6,934 kg/hr (0.214 equivalence ratio). The HRSG unit uses 10,487 kg/hr of steam at a 1:1 syngas/HRSG steam ratio. Validation is carried out against operating conditions for the gasification unit for run #14 from Wei et al. (2009), shown in our previous study (Wilkes, et al., 2021).

Table 1 highlights the KPIs for the BECCS-to-H2 process and Table 2 shows the KPIs for the BECCS-to-SAF process. The BECCS-to-H2 process has higher thermal energy output, as H2 is more energy dense than hydrocarbon fuels (on a mass basis). In both cases the energy demand for the CO2 separation process (1050 kW) is 6% of the total biomass energy input. Figure 3 highlights the fuel/H2 efficiency and product flowrates for the two processing routes. Focusing only on fuel efficiencies, the production of hydrogen from biomass is 36% efficient compared to 19% for Jet Fuel production, which increases to 32% with the inclusion of gasoline and diesel fractions. In both cases the additional power generated from the HRSG improves the energy efficiency, to almost 50% in BECCS-to-H2 and 47% in BECCS-to-SAF if all FT fuels are considered (see Table 1 and Table 2). The results highlight the improved efficiency when incorporating BECCS into BtX processes.

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| Table 1: BECCS-to-H2 KPIs   |  |  | | --- | --- | | **KPI** | **BECCS-to-H2** | | Power demand (kW) | 1,475 | | Power generated (kW) | 3,846 | | Net power output (kW) | 2,371 | | Hydrogen output (kg/hr) | 185.3 | | Hydrogen output (kW) | 6,176 | | Electrical efficiency (%) | 13.80 | | (%) | 35.94 | | Net efficiency (%) | 49.74 | | Table 2: BECCS-to-SAF KPIs   |  |  | | --- | --- | | **KPI** | **BECCS-to-SAF** | | Power demand (kW) | 1,274 | | Power generated (kW) | 3,846 | | Net power output (kW) | 2,572 | | Gasoline output (kg/hr) | 88.50 | | Jet fuel output (kg/hr) | 275.6 | | Diesel output (kg/hr) | 99.40 | | Total fuel output (kg/hr) | 463.4 | | Total fuel output (kW) | 5,510 | | Electrical efficiency (%) | 14.97 | | (%) | 19.06 | | (%) | 32.06 | | Net SAF efficiency (%) | 34.03 | | Net Fuel efficiency (%) | 47.03 | |

Overall, the net efficiency is higher in the BECCS-to-H2 process; however, the BECCS-to-SAF process produces 150% more product (on a mass basis). Despite the lower efficiency, higher profits could be achieved depending on the cost associated with the FT equipment. Hence, a full techno-economic assessment is required to compare these two biomass utilization pathways.

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| Figure 3: Fuel efficiency and production flowrate for BECCS-to-H2 and BECCS-to-SAF |

# Conclusion

Bioenergy with Carbon Capture and Storage (BECCS) and biomass-to-X (BtX) can be combined into BECCS-to-X, a pathway to convert biomass resources into both power and useful products. This paper focuses on the production of hydrogen (H2) and sustainable aviation fuel (SAF). Herein, BECCS-to-H2 and BECCS-to-SAF processes are evaluated and compared using process model developed in Aspen Plus. The study highlighted key operating parameters and performance indicators. Interestingly, producing H2 results in a higher energy conversion, 15.71% points higher than SAF and 2.71% points higher than all FT fuels combined. However, on a mass basis more product is produced in BECCS-to-SAF, hence an economic study is required to ascertain the most cost-effective pathway.

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