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Evaluation of Miscanthus Gasification And Oxy-combustion Carbon Dioxide Removal Potential With Carbon Capture Towards Implementation Of Bioenergy With Carbon Capture And Storage In England

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**Abstract**

Bioenergy with Carbon Capture and Storage (BECCS) pathways and supply chain designs are researched broadly and implemented for scenarios as of the IEA's (2021) Net Zero by 2050 report. The Committee on Climate Change (2018a, 2018b) has identified Miscanthus as one biomass type to achieve its negative emission goals and aligned one third of 1.2 million hectares under high level and one third of 0.7 million hectares under medium level of ambition (multi-functional land use) for the cultivation of Miscanthus for BECCS in the UK.

In this study the input of 39 t/hr of Miscanthus x giganteus biomass as well as Energy technologies institutes (2015) information on projected distributed BECCS installations in the UK for BECCS were considered to bring up different gasifying agent options for H2 generation through Miscanthus Gasification with pre combustion carbon capture and one configuration for oxy-combustion with post combustion carbon capture for highly efficient power generation. Process simulations with Aspen software were conducted to determine power yields and carbon capture rates of optimized bioenergy with carbon capture value chains, sensitivity analysis were executed in order to optimize the configurations.

The aim of the study was to observe how highest achievable power generation efficiencies of H2 generation through gasification of Miscanthus x giganteus compare with oxy-combustion power generation efficiency and how the different pathways influence the carbon capture efficiency. The aim was to inform BECCS implementation decisions with optimum possible H2 and power generation yields as well as their respective carbon capture potential.

It was found that under oxygen, air and steam as gasifying agents steam is most effective for H2 generation with 3.1 t/hr of H2 produced under a input of 39 t/hr of Miscanthus input, which generates 35,6 MW of power in a simulated H2 turbine. Under simulation assumptions it captures thereby 55,2 t/hr of CO2 with a carbon capture rate of 99%. Oxy-combustion is more efficient than the gasification pathways in regard of power generation, which is 100,4 MW with CO2 capture of 36,6 t/hr with an carbon capture efficiency of 73,8 %.

Concluding oxy-combustion is preferred, if highly efficient power generation is wanted and lower carbon capture rate is accepted thereby. When H2 generation is preferred, steam gasification should be
chosen as highest efficient gasification pathway. The exact numbers of power generation as well as carbon capture can be used now to estimate UK’s overall power generation as well as carbon capture potential of Miscanthus x giganteus cultivation under different land use scenarios considering land use change effects and biodiversity.

**Introduction**

The Committee on Climate Change (CCC) of the UK states biomass as most beneficial to both store carbon and displace fossil fuels (Committee on Climate Change 2018a, p.24). In its ”Land use: Reducing emissions and preparing for climate change” report it assumes 1.2 million hectares under high level and 0.7 million hectares under medium level of ambition (multi-functional land use) by 2050 for the evenly split across the three crop types Miscanthus, Short Rotation Coppice Willow and Short Rotation Forestry (Committee on Climate Change 2018b, p.45). For Miscanthus, only combined heat and power (CHP) supply chains have been studied by García Freites, Gough & Röder (2021), while the carbon capture and bioenergy generation efficiency of the aspired gasification to hydrogen and combustion supply chain haven’t been analyzed, especially not with a tailored Miscanthus feed rate as it is adapted in this study from García-Freites, Gough & Röder (2021) and their expert interviews. The aim of the current study is to simulate and compare carbon capture and bioenergy efficiencies of Miscanthus gasification and oxy-combustion supply chains for England in order to compare it with each other.

**Statement of theory**

In this study the input of 39 t/hr of Miscanthus x giganteus input of biomass as well as Energy technologies institutes (2015) information on projected distributed bioenergy with carbon capture and storage (BECCS) installations in the UK for BECCS were considered to bring up different gasifying agent options for H2 generation through Miscanthus Gasification with pre combustion carbon capture and one configuration for oxy-combustion with post combustion carbon capture for highly efficient power generation. Process simulations with Aspen © software were conducted to determine power yields and carbon capture rates of optimized bioenergy with carbon capture value chains, sensitivity analysis were executed in order to optimize the configurations.

**Ultimate Analysis**

Ultimate Analysis after García-Freites, Gough & Röder (2021) is shown in Table 1.

*Table 1 Proximate analysis (dry basis) of Miscanthus in shares (%) after García-Freites, Gough & Röder (2021)*

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<th>Ultimate Analysis after</th>
<th>García-Freites, Gough &amp; Röder (2021)</th>
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<tr>
<td>Carbon</td>
<td>45.1 %</td>
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<tr>
<td>Hydrogen</td>
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<tr>
<td>Oxygen</td>
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Thermodynamic equilibrium approach

Thermodynamics is according to Drake (2021b): “[…] science of the relationship between heat, work, temperature, and energy. In broad terms, thermodynamics deals with the transfer of energy from one place to another and from one form to another. The key concept is that heat is a form of energy corresponding to a definite amount of mechanical work.” Thermodynamic equilibrium is according to Britannica (2018): “condition or state of a thermodynamic system, the properties of which do not change with time and that can be changed to another condition only at the expense of effects on other systems. For a thermodynamic equilibrium system with given energy, the entropy is greater than that of any other state with the same energy. For a thermodynamic equilibrium state with given pressure and temperature, the Gibbs free energy is smaller than that of any other state with the same pressure and temperature.”

Entropy is according to Drake (2021a): “[…], the measure of a system’s thermal energy per unit temperature that is unavailable for doing useful work. Because work is obtained from ordered molecular motion, the amount of entropy is also a measure of the molecular disorder, or randomness, of a system.” Britannica (2012) defines free energy as: “in thermodynamics, energy-like property or state function of a system in thermodynamic equilibrium. Free energy has the dimensions of energy, and its value is determined by the state of the system and not by its history. Free energy is used to determine how systems change and how much work they can produce. It is expressed in two forms: the Helmholtz free energy F, sometimes called the work function, and the Gibbs free energy G. If U is the internal energy of a system, PV the pressure-volume product, and TS the temperature-entropy product (T being the temperature above absolute zero), then F = U − TS and G = U + PV − TS. The latter equation can also be written in the form G = H − TS, where H = U + PV is the enthalpy. Free energy is an extensive property, meaning that its magnitude depends on the amount of a substance in a given thermodynamic state.”

Thermodynamic equilibrium approach in Aspen © modelling refers to the way in which the reaction proceeds. In this case, the biomass will decompose by minimizing the Gibbs energy. This can be done by using the RGIBBS model of Aspen Plus © to simulate the reactor. In Aspen Plus © the modelling of the reactor depends on the mechanism of the reaction and the specific type of the reactor (f.e. Circulating fluidized bed gasifier) has to be taken into account for economics and utilities. An algorithm for the approximation of downdraft gasification product gas compositions must be based on the chemical equilibrium between its different reaction species. Therefore, several assumptions are necessarily made as an infinite residence time such that the pyrolysis products burn and achieve thermodynamic equilibrium in the reaction zone prior to exiting the gasifier (Samson et al. 2018). Furthermore, its products are tar free and assumed to behave as ideal gases and only include H2, CO, CO2, CH4 and N2 (Altafini, Wander & Barreto 2003; Zainal et al. 2001). To describe and study the most significant parameters influencing a gasification process, equilibrium data can be utilized (Schuster et al. 2001; Zainal et al. 2001). Based on the elemental analysis of the Miscanthus biomass, the molecular weight of the fuel can be estimated (Samson et al. 2018).

Based on different literature (Kuo & W. Wu 2015; Ahmad et al. 2011; Sharmina Begum, M.G. Rasul & Delwar Akbar 2014; S.M. Beheshti, H. Ghassemi & R. Shahnasav Markadeh 2015; Frédéric Paviet, Florent Chazarenc & Mohand Tazerout 2009; Andrés Melgar et al. 2007; Mehrdokht B. Nikoo & Nader Mahinpey 2008; Aitziber Erkiaga et al. 2014), the following assumptions were considered to implement the simulation of the gasification system presented after Islam (2020).

• All the parameters are at steady state
• No pressure loss occurred in the system
• All the reversible reactions reached equilibrium
• Although the biomass devolatilization process was instantaneous, the residence time was long enough to reach equilibrium
• All gases were ideal gases
• The particle size has minor or no significant influence on the syngas compositions
• No tar or ash was formed
• The fluidization regime consisted of only of the two regions bed and freeboard.

The gasification operation was isothermal separately for the two regions in the higher temperature bed and the lower temperature freeboard In the published literature, Aspen © simulation of gasification with a complete equilibrium approach generally consists of one RSTOIC, one RYIELD reactor, and one or two GIBBS reactors according to Islam (2020). In considering the chemical equilibrium, several assumptions are made, which include an infinite residence time such that the pyrolysis products burn and achieve thermodynamic equilibrium in the reaction zone prior to exiting the gasifier. Additionally, the products are tar free and assumed to behave as ideal gases, which only include H₂, CO, CO₂, CH₄ and N₂ (Zainal et al. 2001; Altafini, Wander & Barreto 2003). Equilibrium data can be utilized thereby to describe and study the most significant parameters influencing a gasification process (Schuster et al. 2001; Zainal et al. 2001) according to Samson et al. (2018). Redlich-Kwong-Soave equation with Boston-Matias modifications is used as thermodynamic method to describe the interaction between particles of different as well as same substances.

Gasification with pre combustion carbon capture and hydrogen generation

Gasification involves the conversion of a solid fuel into a gas through partial oxidation at temperatures between 750 °C and 1,000 °C (Samson et al. 2018). According to Mutlu & Zeng (2020) gasification is defined as thermochemical conversion of carbonaceous materials into combustible gases, which is generally performed between 600 °C - 1500 °C in the presence of steam, air, O₂, CO₂ or the mixture of these gases are use case dependend (Motta et al. 2018; Shah, Gou & J. Wu 2019). The main product of a typical gasification process, known as syngas, consists of a mixture of H₂, CO, CO₂, CH₄, N₂, H₂O as well as other light hydrocarbons (Kaushal & Tyagi 2017). Gasification process consists of different steps including drying, devolatilization, and pyrolysis, partial oxidation, referred as combustion, of volatiles and the remaining char. Biomass gasification takes place in reactors called gasifiers, which are categorized by different criteria such as the type of the gasification environment, bed material, heat supply source, and the characteristics of the fluid mechanics inside the bed. Each gasifier type has a own design, construction and operational characteristics along with different application areas (Anukam et al. 2016; Susastriawan, Saptoadi & Purnomo 2017). Gasification is a complex process in which chemical reactions as well as heat and mass transfer mechanisms take place. Many parameters such as the feedstock type, gasifier configuration, gasification agent, temperature, and pressure can affect the operational performance and the syngas quality (Mutlu & Zeng 2020). According to Xue et al. (2014) the equivalence ratio is defined as the ratio between the amount of O₂ fed to the gasifier and the O₂ needed for a complete stoichiometric combustion of a unit mass of biomass. Their definition of gas yield is the ratio of the mass flow rate of total N₂-free product gas to the mass flow rate of dry, ash-free biomass, which is also an important parameter for evaluating the performance of gasification processes.

As Kamble et al. (2019) states tar content of the producer gas influences combustion engines and gas turbines due to possible system blockades caused. The gasification process consists of a series of exothermic and endothermic reactions according to Islam (2020) following Emami Taba et al. (2012), Formica, Frigo & Gabrielli (2016), Fu et al. (2011), M. S. Hussein et al. (2017), Kuo & W. Wu (2015), Pala et al. (2017), and Renganathan et al. (2012):
• Drying: $\text{H}_2\text{O (l)} \rightarrow \text{H}_2\text{O (g)} - 40.7 \text{kJ mol}^{-1}$
• Devolatilization: $\text{CHxOyNz (biomass)} \rightarrow \text{Char} + \text{Volatile matters}$
• Char partial combustion: $2\text{C} + \text{O}_2 = 2\text{CO} + 268 \text{kJ mol}^{-1}$ • Partial oxidation: $\text{C} + \text{O}_2 = \text{CO}_2 + 406 \text{kJ mol}^{-1}$
• Boudourad: $\text{C} + \text{CO}_2 \rightarrow 2\text{CO} - 172 \text{kJ mol}^{-1}$
• Water - gas (primary): $\text{C} + \text{H}_2\text{O CO} + \text{H}_2 - 131 \text{kJ mol}^{-1}$
• Water - gas (secondary): $\text{C} + \text{H}_2\text{O CO}_2 + \text{H}_2 + 42 \text{kJ mol}^{-1}$
• Water - gas shift (WGS): $\text{CO} + \text{H}_2\text{O CO}_2 + \text{H}_2 + 42 \text{kJ mol}^{-1}$
• Methanation: $\text{C} + 2\text{H}_2 \rightarrow \text{CH}_4 + 75 \text{kJ mol}^{-1}$
• CO partial combustion: $2\text{CO} + \text{O}_2 = 2\text{CO}_2 - 568 \text{kJ mol}^{-1}$
• H2 partial combustion: $2\text{H}_2 + \text{O}_2 = 2\text{H}_2\text{O} - 484 \text{kJ mol}^{-1}$
• Steam - methane reforming: $\text{CH}_4 + \text{H}_2\text{O CO} + 3\text{H}_2 - 247.4 \text{kJ mol}^{-1}$
• Dry reforming: $\text{CH}_4 + \text{CO}_2 \rightarrow 2\text{CO} + 2\text{H}_2 - 247.4 \text{kJ mol}^{-1}$ • Thermal cracking: $\text{CnH}_m \rightarrow \text{C} + \text{CxHy} + \text{H}_2$
• H2S formation: $\text{H}_2 + \text{S} \rightarrow \text{H}_2\text{S} + 20.2 \text{kJ mol}^{-1}$
• NH3 formation: $\text{N}_2 + 3\text{H}_2 \rightarrow 2\text{NH}_3 + 92 \text{kJ mol}^{-1}$

Because of its high energy efficiency and improved environmental performance compared to direct combustion, gasification is seen as a good alternative (Kirkels & Verbong 2011; Pereira et al. 2012; Xue et al. 2014). Furthermore it also has the potential to be applied for chemicals as well as fuel production (Kirkels & Verbong 2011). The main components of the producer gas are CO, H2, CH4, N2, and CO2 (Kuo, W. Wu & Chen 2014; Xue et al. 2014). This producer gas can be directly combusted or can be further upgraded for the production of chemicals and fuels. Gas composition is affected by several factors as the type of biomass feedstock utilized, type of gasifier utilized, the gasifying agent, residence time, and also the temperature of the process (Heidenreich & Foscolo 2015). The producer gas contains impurities such as tars, particulates, nitrogen and sulfur compounds (Galindo et al. 2014). Gasification is highly flexible in terms of feedstock materials (Heidenreich & Foscolo 2015). Hodgson, Lister, et al. (2010) showed in a European Miscanthus study that Miscanthus giganteus has a high lignin content, compared with other biomass crops, which is advantageous for thermochemical conversion due to its higher energy content when compared with cellulose and hemicelluloses (Demirbaş 1997; Friedl et al. 2005; Hodgson, Nowakowski, et al. 2011). It has also been shown to have low mineral content and high efficiency of carbon sequestration above and below ground (Xue et al. 2014). According to Samson et al. (2018) most Miscanthus gasification studies have been performed on small, laboratory-scale, reactors, and little information could be found for pilot-scale work in fixed bed reactors (Simone et al. 2012). Samson et al. (2018) successfully applied thermodynamic equilibrium modelling to a pilot-scale gasification process and showed that simple equilibrium modelling methods can be utilized to predict gas compositions for the pilot scale.

**Oxy-combustion**

Oxy-fuel combustion is a combustion process with the removal of nitrogen from the oxidizer. The share of oxygen in the oxidizer is higher than in air and therefor over 21%. Oxy-fuel combustion recycles flue gas to achieve a lower flame temperature, which makes it a highly efficient combustion technology (Z. Wang 2018). Yaverbaum (1977) brought up the concept of oxy-fuel combustion. Pure oxygen is used instead of air to obtain high concentrations of CO2. Part of the flue gas is required to be recirculated in order to control the temperature of furnace flame and maintain appropriate characteristics of heat transfer. As biomass combustion with oxygen leads to higher temperatures, special materials are necessary to withstand such temperatures, increasing the overall costs. Hence, recycling flue gas allows reducing the oxygen concentration leading to lower temperature. The process benefits for CO2 capture and compression. Oxy-fuel combustion technology was first applied to pulverized coal-fired boiler. Because of high power consumption on the application of oxygen-rich combustion the focus of oxy-fuel
combustion technology changed to circulating fluid bed boiler. Oxy-fuel combustion key technologies have been tested and matured, whereas research on oxy-fuel combustion technology of circulating fluidized bed is out of the laboratory stage (Z. Wang 2018). Oxy-fuel combustion is considered to have high potentials for carbon dioxide capture. In much of the literature on the oxy-fuel process, the combustion conditions are optimized to be similar to those in a traditional air-fired process. The new technology could therefore be easily transferred to conventional furnaces (Z. Wang 2018). To obtain temperature levels similar to those in conventional combustion, part of the flue gas is recirculated (Normann et al. 2008). The high CO2 concentrated flue gas is discharged from the tail of the boiler and purified by a flue gas cleaning system before it enters the compression and purification unit to obtain high purity liquid CO2 for transportation, utilization, and storage (Z. Wang 2018).

Oxy-fuel combustion has the following advantages (Z. Wang 2018):

• High flame temperature and blackness
• Improves the burning speed, promote safety of combustion
• Reduces the ignition temperature of the fuel and the burnout time
• Reduce the excess air coefficient, and the amount of flue gas after combustion More competitive compared to the other CO2 control technologies
• Both suited for new boilers, and the transformation of old boilers
• Significantly beneficial for NOx reduction
• Provides a new way for the integration of other pollutants’ control technologies Oxy-combustion involves burning fuel in a mixture of recycled CO2 and pure O2 instead of air and it results in a flue gas that is composed mainly of CO2 and water vapour.

This flue gas can be easily separated at low cost by a condensation process. In oxycombustion the oxygen production is a costly and energy intensive process, typically done by cryogenic air separation. The potentials lie in high CO2 separation efficiencies and relative simplicity of the method (Florin & Fennell 2010). Oxy-combustion means higher temperatures due to using a high Equivalence Ratio of O2, the product gas has a high CO2 concentration in conclusion. The Clausius-Rankine-Cycle works by closed circuit, which alternately evaporates by adding heat at high pressure and condenses after expansion while releasing work by removing heat at low pressure.

Carbon capture

BECCS supply chains offer different technological pathways to produce electricity, heat or biofuels. In the power sector, BECCS applications are typically categorised by one of three broad CO2 capture methods: post-combustion, pre-combustion and oxy-combustion, which the other way around depend on the bioenergy conversion technology (Daggash et al. 2019). Selexol is a physical solvent. Physical solvents have a higher absorption capacity, suitable for syngas containing higher CO2 concentrations and are preferred for CO2 capture when the gas has higher partial pressures of CO2 at the inlet of the absorption process (Jansen et al., 2015). In carbon capture through physical absorbents like Selexol CO2 is physically absorbed in a solvent following Henry’s Law, which means that the physical absorber is temperature and pressure dependent. It uses Selexol as organic solvent to physically absorb acid gas components rather than reacting chemically. Removal of CO2 is based on the solubility of CO2 within the Selexol and the solubility depends on the partial pressure and the temperature of the feed gas. Higher CO2 partial pressure and lower temperature thereby favour the solubility of CO2 in the absorbing Selexol, which is regenerated by either heating or pressure reduction (Johnson & Homme, Jr, A C 1984). The interaction between CO2 and physical absorbents is weak relative to chemical solvents, decreasing the energy requirement for regeneration. Selexol (dimethyl ether of polyethylene glycol) is a liquid glycol, which is effective for capturing CO2 at higher concentration (Olajire 2010).
According to Olajire (2010) the advantages of Selexol process are:

• The heat rise of the solvent in the absorber is low (no heat of chemical reaction)
• The sweet gas from the absorber comes out dry (high affinity of Selexol solvent with water)
• The initial plant and operating costs are very low
• Regeneration of the solvent is by air stripping, which requires no re-boiler’s heat
• Selexol process allows for construction of mostly carbon steel (non-aqueous and inert chemical characteristics)
• The process could be operated at low pressure

While according to Olajire (2010) the disadvantages of Selexol process are:

• The solvent has high affinity to heavy hydrocarbon, which will be removed with CO2 and essentially result to hydrocarbon losses
• The process is more efficient at high operating pressure CO2 dissolved in the solvent is recovered by reducing pressure in various flash drums.

No heat is required to release CO2 due to the low heat of absorption. After depressurization, pure CO2 streams are released at different pressures (Olajire 2010). Post-combustion capture involves the separation of CO2 from flue gas after a fuel combustion process by applying chemical absorption methods. It can be retrofitted from existing power plants and is the most mature and currently deployed technology (Florin & Fennell 2010). Pre-combustion CO2 capture is associated with gasification or steam methane reforming. A producer gas, comprised mainly of carbon monoxide, hydrogen, methane and CO2 is produced and subsequently reacted with steam to produce a shifted gas containing mainly CO2 and H2. The CO2 is then separated typically using physical absorption methods (Jansen et al. 2015). Oxy-combustion capture entails the CO2 separation from flue gas, which is mainly composed of CO2 and water vapour via a condensation process. This flue gas composition results from burning fuel with oxygen and recycled CO2 (Florin & Fennell 2010). Oxyfuel combustion is a modified post-combustion method. The fuel is combusted in almost pure oxygen instead of air, which results in high concentration of CO2 in flue gases. CO2-rich flue gas is thereby recycled to the combustor to make the flame temperature similar to normal air-blown combustors as O2 increases the temperature strongly. The high CO2 purity as well as NOx formation suppressing is beneficial. The physical separation processes for O2 production and CO2 capture avoid the wide use of any reagent and solvents. The main disadvantage of oxyfuel combustion is the large quantity of expensive oxygen required (Olajire 2010).

Knowledge gaps exist for what combination of biomass, energy conversion and carbon capture technologies and final energy vectors will deliver most effective BECCS supply chains (Daggash et al. 2019; ETI 2016; IEA Bioenergy 2020). To deploy BECCS successfully the implications of the full supply chain, from biomass production to CO2 storage, needs to be understood from an emission, engineering, economic, social and policy point of view according to García-Freites, Gough & Röder (2021).

Description and Application of Equipment and Processes

Aspen Plus © is used as a chemical process modelling software, being flexible regarding different process configurations, which allows to optimize varying operational conditions and determine limitations of its processes (Mutlu & Zeng 2020). The Equilibrium approach of modelling, classified as non-stoichiometric, is applied by assuming ideally mixed reactants, which react with each other in an infinite period of time (Mutlu & Zeng 2020). The non stoichiometric modelling approach, based on
minimization of the Gibbs free energy, advantage is that it requires almost no details of the system for the process description and the prediction of its outcome (De et al. 2018). Equilibrium modelling is performed using RGibbs blocks which is based on the minimization of the Gibbs free energy of the system in terms of the mole numbers of the species present in all phases, i.e., reactants, product (D. Baruah & D. C. Baruah 2014; Basu 2018; Kuo, W. Wu & Chen 2014). A steady-state, isothermal process with a homogeneous temperature and pressure profile, and no pressure drops inside the reactor is assumed allowing the reactants to reach the equilibrium state (Adelayemi & Janajreh 2015; Damartzis, Michailos & Zabaniotou 2012; Dhanavath et al. 2018; Kuo, W. Wu & Chen 2014; Mutlu & Zeng 2020). It is assumed during biomass decomposition, that yield and composition of the devolatilization products can be derived from ultimate and proximate analysis of the fuel (Damartzis, Michailos & Zabaniotou 2012; Han et al. 2017; Kaushal & Tyagi 2017; Mutlu & Zeng 2020). Therefore it is important to understand the properties of the selected fuel as well as the requirements of the gasification and combustion process and compare for example syngas compositions with the literature (Mutlu & Zeng 2020). As handling tar formation during gasification processes is still one of the biggest challenges in modelling and to simplify, tar formation is not included at all or considered assuming the formation of an inert compound (Begum et al. 2014; Linköping University Electronic Press 2015).

**Miscanthus Gasification**

Miscanthus with a feed rate of 39 t/hr as well as an oxidizing agent (O2, Steam, Air (N2 free)) is fed into a heated R-Gibbs Gasification Reactor (Figure 1). The exhaust is separated into char (ash) and syngas, which is enriched by heated steam 400 °C hot. In another R-Gibbs reactor the steam added syngas follows a water gas shift reaction, which fluegas is cooled down in a Flash reactor in order to separate the water and recycle it back into the steam circle, while 10% of the water is renewed in order to avoid accumulation of traces. The drygas consisting mainly out of CO2 (98%) and some H2, N2, H2O, CO and CH4 in descending order is passed to the Selexol carbon capture. The Hydrogen is streamlined into a Brayton circle (figure 2.3), where it gets mixed with heated, compressed air in order to combust the mixture and fire a Gas turbine.

![Figure 1 Flowsheet of Gasification with O2 as a gasifying agent](image)

**Oxy-combustion**

Miscanthus with a rate of 39 t/hr added by O2 mixed with recycled CO2 is fed into boiler. The heated fluegas is streamlined through a heat exchanger, which is also streamlined of a water-steam stream, which runs a steam turbine and therefore produces work. After the heat exchanger the ash is separated from the fluegas, which is cooled down in order to remove water. The resulting drygas feeds back into
the oxyifying stream. The drygas is fed in a share into the selexol carbon capture process (Figure 2).

**Figure 2 Flowsheet of Oxy-combustion pathway**

**Carbon capture**

The fluegas from the gasification process is compressed and heated before it gets fed into an absorber, which is fed by a liquid Selexol stream. For oxy-combustion heated fluegas is fed into the absorber. This absorber functions for H2 as a pressure swing adsorbtion under the thermodynamic method of PC – saft. It recovers and purifies the H2 share of the fluegas with a recovery rate of 70% of H2 with a purity of 88%. The remaining fluegas is send through multiple turbines, valves and flash reactors in order to reduce the pressure and therefore temperature efficiently, so CO2 can be separated from the Selexol (CO2 gas, Selexol liquid). With this process CO2 can be recovered in a purity of 99%. The fluegas stream resulting after the first turbine and flash reactor, consisting out of CO2, H2O, H2 and CO is recycled back into the fluegas resulting from the gasification. The remaining Selexol stream, including the traces, gets renewed with 20% in order to avoid accumulation of the traces. It is compressed to the required pressure and temperature of the absorption and send back into the absorber (Figure 3).

**Figure 3 Flowsheet of Selexol carbon capture**
Sensitivity Analysis

In the sensitivity analysis equivalence ratio, gasifier temperature, pressure, feed flowrates, feed compositions, preheating conditions, and steam flow rates are varied as in Islam (2020). According to Islam (2020) the gasification temperature is an important factor that influences the gas compositions, tar yield, and other performance parameters. The gasification temperature increases with an increasing equivalence ratio (Islam 2020). The Sensitivity Analysis was proceeded with optimizing the power yields as first prioritization and optimizing the carbon capture rates as second prioritization within the boundaries of literature recommended parameters, while showing the impact of extending these in the sensitivity analysis itself. Ikhlas Ghiat et al. (2020) recommend a gasifier temperature between 600 °C and 1000 °C. Values of parameters were oriented at these values, but extended widely for the sensitivity analysis of this study. The gasifying agent flow rate for steam is recommended to be in a range between 20 t/hr and 120 t/hr adjusted to the biomass input in this study (Huang & Jin 2019). For O2 it is defined at 11.7 t/hr derived from Tauqir, Zubair & Nazir (2019), while for Air it can be derived as well as its O2 share is known. Gasifying agents such as air, oxygen, steam, CO2, or their combinations can influence several of the above-mentioned reactions according to Le Chatelier’s principle and increase the concentration of H2 and CO in the syngas (Islam 2020). In Aspen © simulations air behaves identical to oxygen as gasifying agent except that N2 as an inert doesn’t take part in the reactions. Introducing pure oxygen influences the rate of the several endothermic reactions according to Islam (2020). It is expensive due to the substantial amount of compression and refrigeration work required for oxygen separation from the air (Islam 2020). Liu et al. (2018) experimentally showed that the CO2 concentration is higher than CO for biomass gasification in the fluidized bed gasifier with an oxygen-enriched reactant. Oxygen thereby increases flame temperatures. Steam has been studied as an oxidant for improving the quality of syngas in other studies as Dharminder Singh et al. (2020). Oxygen with steam was used to produce syngas that would overcome the issue of dilution of syngas by nitrogen commonly encountered during air gasification (Lv et al. 2007; Carpenter et al. 2010) according to Islam (2020). The addition of steam as gasifying agent and catalyst in gasification process makes it possible to obtain high-grade products from gasification of Miscanthus in catalytic conditions for production of syngas according to Michel et al. (2007). The water input for water gas shift reactor with 4 t/hr and a H2O to CO ratio of 4.2 is taken from Augustine, Ma & Kazantzis (2011) as initial value to start sensitivity analysis. The oxygen to CO2 flow rate ratio of 1:4.2 as well as the CO2 recycle rate of 0.7 is derived from Bailera M., Lisbona P & Romeo L. M. (2015), Kosowska-Golachowska et al. (2016), and A. Hussein & Naser (2013), while boundaries of sensitivity analysis are reached. The oxy-combustion boiler operating temperature of 1400 °C is derived from Xiang et al. (2019), while the mass flow rate of the water for the steam turbine as well as the pressure of pumping the water are derived from Khallaghi et al. (2021).

Presentation of Data and Results

Sensitivity Analysis

The Hydrogen generation with steam as a gasifying agent reaches in its product gas composition a plateau from a steam input rate of 40 t/hr (Figure 5) and a plateau at a gasifier temperature of 650 °C (Figure 4). The increase of generated power through increasing WGS temperatures reaches a plateau around a WGS reactor temperature of 400 °C (Figure 6). The power yield for varied steam input rates reaches a plateau from a steam input rate of 40 t/hr (Figure 7).
Figure 4 Gasification product gas composition with steam as gasifying agent after different gasifier temperatures for input rates of 39 t/hr

Figure 5 Gasification product gas composition with steam as gasifying agent after different steam input rates for 39 t/hr of Miscanthus input
Figure 6 Power yield and Carbon capture after different WGS reactor temperatures with steam as a gasifying agent with an input rate of 39 t/hr of Miscanthus.

Figure 7 Power yield and carbon capture per steam input rate for gasification of 39 t/hr of Miscanthus.

The Hydrogen generation with O₂ as a gasifying agent reaches in its product gas composition peak for hydrogen at a O₂ input rate of 9 t/hr (Figure 10) and a plateau at a gasifier temperature of 700 °C (Figure 8). The increase of generated power through increasing WGS temperatures reaches a plateau around a WGS reactor temperature of 400 °C (Figure 9). The power yield is highest for a O₂ input rate.
of 0 t/hr and falls from a O2 input rate of 9 t/hr onwards (Figure).

Figure 8 Gasification product gas composition with O2 as gasifying agent after different gasifier temperatures for input rates of 39 t/hr of Miscanthus

Figure 9 Power yield and Carbon capture after different WGS reactor temperatures with O2 as a gasifying agent with an input rate of 39 t/hr of Miscanthus
The Hydrogen generation with Air as a gasifying agent reaches in a product gas composition plateau at a steam input rate of 40 t/hr (Figure 11) and a plateau at a gasifier temperature of 700 °C (Figure 10). The increase of generated power through increasing WGS temperatures reaches a plateau around a WGS reactor temperature of 400 °C (Figure 12). The power yield declines from a Air input rate of 0 t/hr onwards (Figure 13).
Figure 102 Gasification product gas composition with Air as gasifying agent after different gasifier temperatures for input rates of 39 t/hr of

Figure 113 Gasification product gas composition with Air as gasifying agent after different O2 input rates for 39 t/hr of Miscanthus input
Maximum power yields as well as carbon captured is reached for oxy-combustion at a oxygen input rate of 38 \( t/hr \). Sensitivity analysis with higher oxygen input rates were not possible to process with Aspen ©. A parameter value of 38 \( t/hr \) (Figure 15), which represents a equivalence ratio of 0.67 was chosen for further analysis. The highest possible to simulate boiler temperature of 1400 °C resulted in the highest power yield, while the carbon capture rate decreased simultaneously for oxy-combustion simulations (Figure 14). The power generation for oxy-combustion for the parameter of water input into the steam turbine peaks at 60 \( t/hr \) of water input into the steam turbine (Figure 16). The increase of initial pressure of the steam turbine from 25 bar onwards leads to continuously increased power yields, peaking at 100 bar (Figure 17).
Figure 146 Power yield and carbon capture per O2 input rate for gasification of 39 t/hr of Miscanthus

Figure 157 Power yield and carbon capture per oxygen input rate for oxy-combustion of 39 t/hr of Miscanthus
Figure 168 Power in MW per water input (t/hr of steam turbine for oxy-combustion pathway of 39 t/hr of Miscanthus)

Figure 179 Power in MW per initial pressure of steam turbine for oxy-combustion pathway of 39 t/hr of Miscanthus
Parameter values derived from sensitivity analysis

Air as gasifying agent:
Air is fed with a rate of 40 t/hr representing a equivalent ratio of 0.16. The gasifier temperature is set to 700 °C, while the WGS reactor temperature is set to 400 °C.

Steam as gasifying agent:
Steam is fed with a rate of 40 t/hr representing a equivalent ratio of 0.16. The gasifier temperature is set to 650 °C, while the WGS reactor temperature is set to 400 °C.

Oxygen as gasifying agent:
O2 is fed with a rate of 9 t/hr representing a equivalent ratio of 0.16. The gasifier temperature is set to 700 °C, while the WGS reactor temperature is set to 400 °C.

Oxy-combustion pathway:
Miscanthus with a rate of 39 t/hr as well as 38 t/hr of O2 mixed with recycled CO2 is fed into a 1400 °C hot boiler. The heated fluegas is streamlined through a heat exchanger, which is also streamlined of a water-steam stream, which runs a steam turbine and therefore produces work. After the heat exchanger
the ash is separated from the fluegas, which is cooled down in order to remove water. The resulting drygas feeds back into the oxifying stream with a share of 70%. Because of the oxygen feed the drygas consist mainly out of CO2 (75%), O2 (14%) and CO (10%), which is fed in a share of 30% into the selexol carbon capture process.

From the studies, it was found steam is the most efficient for green hydrogen production. 40 t/hr of steam and 39 t/hr of Miscanthus input produced 3.1 t/hr of hydrogen and generated 35.6MW of power. Under these assumed conditions, Selexol captured 55.2 t/hr of CO2. This accounts for 99% of the total CO2 produced. Furthermore, oxy-combustion has higher overall energy efficiency and generated 41MW for the same input feed rate of Miscanthus and oxygen input of 38 t/hr. However, the carbon capture efficiency at 91.4% was lower, capturing 43.5 t/hr of CO2 under a flue gas recycle rate of 70% (Figure 21).

![Figure 21](image)

**Figure 21** Power yield and Carbon Capture generated through the simulated BECCS Supply Chains with an input of 39 t/hr of Miscanthus for O2 Gasification, Steam Gasification, Air Gasification and for oxy-combustion, with a CO2 recycling rate of 70%

**Conclusion**

Overall, oxy-combustion is preferred compared to gasification, if highly efficient power generation is the objective and lower carbon capture rate is acceptable thereby. On the other hand, if green hydrogen production with carbon capture is preferred, steam gasification should be chosen as highest efficient gasification pathway.

This is the first study analyzing the gasification as well as oxy-combustion BECCS supply chains with Miscanthus as a feedstock through process simulation. These results can inform decision making processes in regard of statement of power generation efficiency as well as carbon capture efficiency, thereby the carbon storage part is not included as well as the life cycle emissions haven’t been considered.
As of the nature of a simulation the analysis depend on simplifications such as the thermodynamic equilibrium.

New simulation runs with different feedstock and different biomass input rates are possible and make the methodology adaptable to other use cases.

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Literature


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