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Integrated plasma gasification and SOFC system simulation using Aspen Plus

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Abstract

Gasification is the thermal decomposition of a solid feedstock into a combustible synthetic gas mainly composed of H_2 and CO. Gasification usually suffers from relatively low electrical efficiencies when coupled with a steam cycle or gas engine power generation trains for electricity generation. The integration of gasifiers with more advanced electricity generation technologies such as Solid Oxide Fuel Cells (SOFC), presents a significant opportunity to maximize the energy recovery from biomass and waste.

This study presents the results of a simulation study, using Aspen Plus, whereby an integrated microwave induced plasma (MIP) gasifier, gas cleaning unit, SOFC and an anode off-gas combustor, was modelled for optimal energy efficiency. MIP gasification is a novel high temperature plasma based advanced thermal conversion technology, that enables generation of a high quality synthetic gas suitable for energy generation using an SOFC. Specific focus has been given to the removal of syngas impurities within the synthetic gas clean-up train to ensure the removal of impurities such as tars, particulates, H₂S and HCI, critical to the performance and durability of the fuel cells.

This study demonstrates the theoretical feasibility of combining MIP gasification and SOFC. The influence of feedstock moisture content on gasification efficiency is investigated showing that best efficiencies are obtained with moisture content close to 21%. The integrated system shows a very high electrical efficiency of up to 34% corresponding to a cell voltage of 0.83 V at low current density and CHP efficiency higher than 70% when turning biomass into electricity.



Introduction

Global warming is the most important concern of the century and must be tackled by reducing greenhouse gas (GHG) emissions. GHG emissions reduction can be achieved by substituting fossil fuels by renewables energy. On the other hand, the amount of waste generated is constantly increasing and efficient waste management options are required to divert waste from landfilling. Waste to energy technology (WTE) is a way to produce value from waste as a fuel resource. In addition, new energy sources are required to face the continuing depletion of fossil fuels that should reach critical levels by the end of the century. Thus, turning waste to energy is a way to face the trilemma of GHG emissions reduction, waste management and depletion of fossil fuels (energy security).

Interest has been shown in the last decade concerning the development of microwave induced plasma (MIP) reactor for waste and biomass gasification [1]. Lupa et al demonstrated the plausibility of using microwave induced plasma (MIP) torch for the thermal treatment of biomass [2] and commercial and industrial waste [3]. MIP gasification is a relatively new and promising technology. In fact, plasma characteristics such as very high temperature improve syngas quality, whereas microwave energy required less electrical energy and has better durability than the more normally utilised Direct Current (DC) electrodes. This study models a demonstrator rig of the gasifier that is currently being developed in the UK by Stopford Energy & Environment, Lancaster University and Liverpool John Moores University.

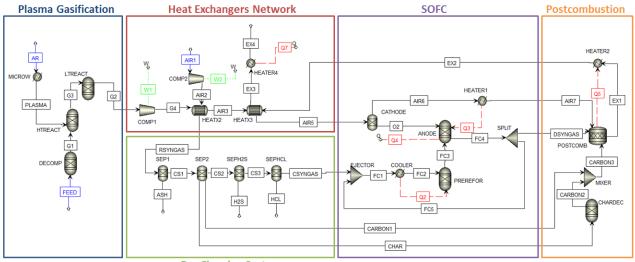
The syngas generated is generally fed to a gas engine or turbine and generator for electricity generation. However, the use of more advanced technology such as Solid Oxide Fuel Cells (SOFC) improves the overall efficiency of the system. On the other hand, SOFC are subject to more stringent requirements in term of pollutants present in gas. Therefore, a gas cleaning system able to reduce the hydrogen sulfide (H₂S), hydrogen chloride (HCl), tars, particles and alkali compounds concentration to very low levels is required.

An integrated gasification and fuel cell system is thus a very promising system enabling an efficient and clean production of electricity from biomass or waste. This study investigates the performance of an integrated system composed of a MIP pyrolyser/gasifier reactor, a gas cleaning unit, an SOFC stack and an anode tail gas burner chamber. The influence of biomass moisture content on the thermal treatment and overall system is investigated while the reactor is operated under pyrolysis condition.

1. Simulations

The whole system composed of a MIP gasifier, a gas cleaning unit, an SOFC and a gas burner has been modelled with Aspen Plus and is represented in Figure 1. The configuration of each unit of the system is described in the following parts.





Gas Cleaning System

Figure 1: Diagram representation of the overall system in Aspen Plus

Plasma Gasification

Plasma gasification is an innovative technology that has some great advantages compared to conventional gasification thanks to the exceptional properties of plasma such as very high temperatures (up to 4,000°C) and high thermal conductivity. Plasma is formed when a high quantity of energy is absorbed by a gas causing its ionization and for MIP microwave is used as a source of energy. Lupa et al published results proving the possibility of pyrolysis using MIP torches [2,3]. A demonstrator rig of the MIP gasifier is currently in development. This demonstrator is composed of three MIP torches producing argon plasma and consuming 0.8 kW each. This rig has been designed to treat a maximum amount of 5 kg/hr of biomass or waste.

The Aspen Plus model of the MIP gasifier has been built on the EquiPlasmaJet (EPJ) model developed by Galeno et al [4]. Modifications to the existing EPJ model have been applied to match the configuration of the MIP gasifier such as reactor temperature.

The MIP gasifier model is first composed of a *RYield* (type of Aspen Plus reactor) reactor (DECOMP in figure 1) that decomposes the feedstock into its elemental components: C, H₂, O₂, N₂, S, Cl₂ and moisture in H₂O. In addition, a part of the H₂ has been forced to be decomposed into methane (CH₄) in order to take its presence in the syngas into account. However, methane had to be defined as inert in the reactors as it will be completely decomposed at reactor temperature when assuming Gibbs free energy minimization method. The gas then enters a high temperature reactor (HTREACT in figure 1) with the argon plasma at 1,000°C. The resulting gas (G3) reaches a chemical equilibrium at a lower temperature of 800°C (LTREACT) corresponding to the gasifier exit temperature of the produced syngas. Those reactors are based on Gibbs free energy minimization method (*RGibbs* reactor type in Aspen Plus) that calculated the equilibrium between chemical species without having to specify the reactions and their kinetics. The main reactions are first the solid carbon oxidation with the decomposed oxygen (1) and steam (2) whereas the water-gas-shift (WGS) reaction (3) is the main reaction in the gas phase:

$C + O_2 \rightarrow CO_2$	(1)
$C + H_2 O \to CO + H_2$	(2)
$CO + H_2O \leftrightarrow H_2 + CO_2$	(3)

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This MIP gasifier model has been validated against experimental results published by Sturm et al [5] where they gasified cellulose using an air plasma. Figure 2 compares the experimental results obtained by Sturm et al with the results obtained with the MIP gasifier model developed in this study. The validation has been carried out at higher temperature of 1,200°C (HTREACT) and 1,000°C (LTREACT) due to the heat released in oxidation reactions as air was used as plasma gas. It is worth noting the high concentration of carbon monoxide compared to carbon dioxide resulting from the high temperature of the plasma leading to backward reaction in the WGS reaction (reaction (3)).

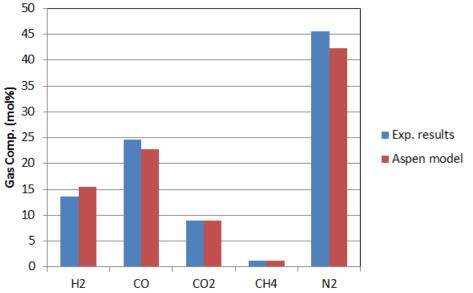


Figure 2: Comparison of MIP plasma gasification syngas composition between experimental results published by Sturm et al [5] and the Aspen Plus model in this study

Gas Cleaning System

The raw syngas generated by the MIP gasifier must be purified in order to meet the stringent requirements of SOFCs in term of gas quality. It is accepted that the HCl, H₂S alkali and particulates concentration should be lower than 1 ppm in order to ensure durable operation of the SOFC [6]. In this study, a modestly elevated temperature cleaning system operating at 400°C is proposed. This system is composed of a cyclone and a ceramic filter for removal of ash and particulates, a sodium carbonate bed for HCl cleaning and a zinc oxide (ZnO) bed for H₂S. The two sorbent beds are modelled using separator removing 99% of the HCl and H₂S of the syngas while the cyclone and ceramic filter remove all the ashes and solid carbon. Tars are not modelled in the simulation but it is expected that plasma gasification results in very low amount of tars in the produced syngas [7].

Solid Oxide Fuel Cells

The SOFC model has been taken from the work of Doherty et al [8]. The syngas is first pre-reformed at a temperature of about 550°C representing the gas temperature entering the SOFC. The reformed gas is then directed to the anode which is modelled as a *RGibbs* reactor in Aspen Plus operating at 910°C where the oxidation of hydrogen, carbon monoxide and methane occurs. The stoichiometric amount of oxygen is transferred from the cathode, modelled as a separator, to the anode in order to give an overall fuel

utilization factor of 0.85. A typical utilization factor of 0.85 has been chosen as it is a high value but not too high so that the concentration losses are limited [8]. A fraction of the depleted gas is then recycled and mixed with fresh syngas before the pre-reformer. The amount of air to the cathode is calculated so that the air utilization factor is equal to 0.167. The air utilization factor is deliberately low to avoid oxygen starvation issue and improve heat recovery from the SOFC [8]. The electron production cannot be modelled in Aspen Plus and the cell voltage is thus calculated in a calculator block according to the equation:

 $V = V_N - \Omega_{Ohm} - \Omega_{Polarisation} - \Omega_{Activation}$

The cell voltage (V) is equal to the Nernst voltage (V_N) minus the ohmic, polarization and activation losses. The calculations of the different parameters are detailed in Doherty et al. [8].

Postcombustion

A burner is implemented in order to recover heat from the combustible gases not oxidized in the SOFC. The combustion chamber is modelled with a *RStoic* reactor type in Aspen Plus where the air outlet of the cathode is used to completely oxidise the remaining combustible gases from the anode outlet of the SOFC and also the solid carbon not gasified in the MIP process.

Heat Exchangers Network

A heat exchanger network is implemented in the integrated system in order to optimize the heat recovery. A heat exchanger (HEATX2) cools down the raw syngas from 800°C to the cleaning temperature of 400°C whilst heating up the inlet air of the SOFC cathode. Another heat exchanger increases the air temperature to 600°C using the exhaust gas from the combustion chamber. Useful heat is then recovered in the heat stream Q7 where this heat can be used for many different applications such as the production of steam.

2. Results

The integrated plasma gasification and SOFC system has been run using wood chip for feedstock with characteristics (proximate and ultimate analysis) taken from Pala et al. [9]. The gasifier is modelled as a pyrolyser in this study, which means that no additional oxidant is entering the gasification chamber. It is expected that, thanks to the exceptional properties of the plasma and the configuration of the reactor, the moisture content in the wood chip is directly turned into steam and act as an oxidant in the reactor. Thus, the moisture content of the feedstock drives the amount of oxidant entering the reactor and is one of the major parameter of the model. Thus, the influence of the moisture content on the system efficiency is first investigated while the flowrate of dry feedstock entering the reactor is kept constant at 5 kg/hr.

Figure 3 presents the different efficiencies obtained for the system as a function of the moisture content of the feedstock. The efficiencies are defined according to the following equations were P_{el} is the AC electrical power produced by the SOFC, P_{magn} and P_{comp} are the electrical power consumed by the magnetrons and the compressors respectively, Q7 is the heat that can be recovered from the system, \dot{m} is a mass flow rate and LHV a lower heating value.

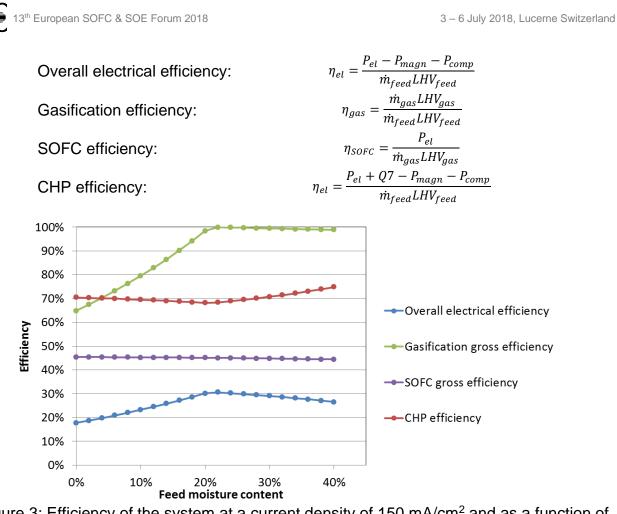
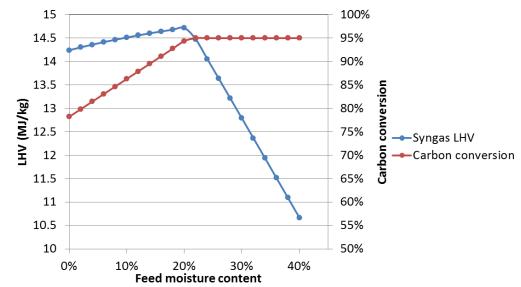
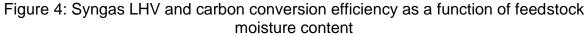


Figure 3: Efficiency of the system at a current density of 150 mA/cm² and as a function of feedstock moisture content

Figure 3 shows that the gasification efficiency is increasing from 65% to 100% while the moisture content is increased from 0% to 21%. A gasification efficiency of 100% means that the same amount of energy is recovered in the syngas that the amount present in the feedstock. This very high efficiency is possible thanks to the characteristics of the plasma that produce a syngas with a high calorific value due to high concentration of hydrogen and carbon monoxide. The increase in efficiency with the moisture content is due to the increase of the carbon conversion efficiency through reactions (1) and (2). In fact, at low moisture, there is not enough oxidant in the reactor to turn solid carbon into carbon monoxide or dioxide, whereas 20% moisture is sufficient to reach the maximum carbon conversion assumed at 95% as shown in figure 4. On the other hand, higher moisture content tends to decrease the calorific value of the gas produced and thus reduced the gasification efficiency (Figure 4). In the same time, higher moisture content results in higher steam concentration in the gas which decreases the SOFC efficiency by 1%. In addition, the model assumes a constant temperature in the plasma reactor whereas an increase in feedstock moisture may results in lower temperature and then lower gasification efficiency due to lower carbon conversion and higher carbon dioxide concentration in the produced gas.





A feedstock moisture content of 21% lead to the highest electrical efficiency of the system with 31% at a current density of 150 mA/cm². The syngas produced with this configuration has a very high quality with:

- 47.1 mol% H₂
- 40.0 mol% CO
- 5.7 mol% Ar
- 2.8 mol% H₂O
- 2.6 mol% CO2

The results displayed in figure 3 are extracted at a current density of 150 mA/cm². However, the current density can be modified varying the area of SOFC while the current is calculated as a function of the amount of combustible gas and the air and fuel utilization factors.

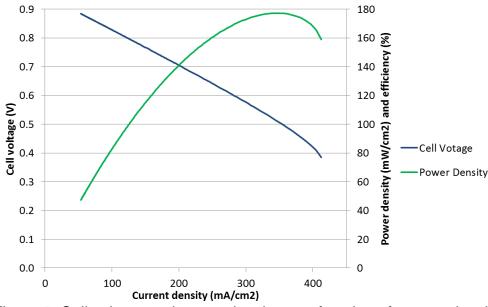


Figure 5: Cell voltage and power density as a function of current density



As shown in Figure 5, the cell voltage obtained is about 0.83 V at a low current density of 100 mA/cm². The cell voltage then decreases rapidly with an increase in current density due to the increase of polarization, activation and ohmic losses. Thus, the cell voltage is reduced to 0.7 V at a current density of 200 mA/cm² which is a usual operation condition for SOFC [8].

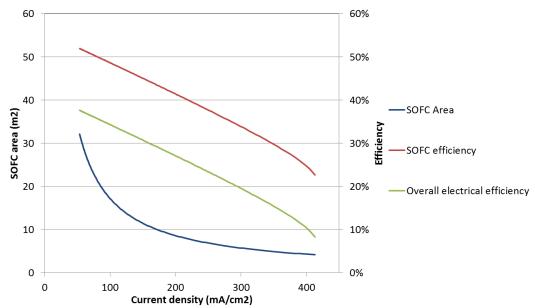


Figure 6: Efficiencies and SOFC area as a function of the current density for a feedstock moisture of 21%

Figure 6 shows that the SOFC efficiency and thus the overall electrical efficiency of the system are decreasing with an increase in current density. The highest efficiencies are then obtained at the lowest current density. On the other hand, low current density is obtained by using a larger number of SOFC cells which means a higher initial cost of the system. There is a compromise to find between the SOFC area and its efficiency. The sizing of the SOFC should be optimized with an economic study. The overall electrical efficiency is varying from 27% to 34% while the current density is reduced from 200 to 100 mA/cm² at a feedstock moisture content of 21%.

Those results are promising as efficiencies higher than 30% can be achieved which is currently the maximum efficiency of gasification power plant when combined with gas engine for power generation [10]. Research and development on SOFC are expected to lead to efficiency improvement so that gasification coupled with SOFC will systematically have higher efficiencies than the use of combustion system. In addition, the SOFC system is more environmentally friendly than combustion devices and thus should be favored in order to reduce CHG emissions.

Conclusion

This study investigates the performance of a system combining MIP gasification and SOFC technologies by means of simulation using Aspen Plus. The moisture content of wood chip must be about 21% in order to optimize the pyrolysis efficiency. The overall electrical efficiency of the system is estimated to be between 27% and 34% corresponding to SOFC cell voltage between 0.7 and 0.83 V for current density varying between 200 and 100 mA/cm². In addition the CHP efficiency of the system is about 70%. This study



demonstrates the theoretical feasibility of the integrated system and confirms the interest in the system due to its high electrical efficiency that is potentially higher than usual combustion system used for electricity generation.

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