Design and system analysis of quad-generation plant based on biomass gasification integrated with district heating

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Quad-generation system

Designing and modelling

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Design and system analysis of quad-generation plant based on biomass gasification integrated with district heating

by

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3. Name and title of supervisor and any other supervisors.

   Lasse Rosendahl, Professor

   Morten B. Blarke. Associate Professor

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   Paper 1: ISI Journal Paper: Rudra, S.; Rosendahl, L; Blarke MB; Proposal of a biomass based Quadgeneration system for power, heat, cooling and SNG production. International journal of green energy (under review)

   Paper 2: Conference paper: Rudra, S.; Rosendahl, L; Hoffmann, J. , Planning of a Quadgeneration power plant for Jammerbugt energy system. Proceedings of the 2nd European Conference on Polygeneration . ed. / Alberto Coronas Salcedo . March, 2011.

   Paper 3: Peer reviewed Conference paper: Rudra, S., Rosendahl, L., & From, N. (2011). Optimization of a Local District Heating Plant Under Fuel Flexibility and Performance, ASME conference proceedings, 1159–1165. 5th International Conference on Energy Sustainability.

   Paper 4: Peer reviewed Conference paper: Blarke, MB; Rudra, S; Rosendahl LA; QUAD-Generation: Techno-Economic Analysis Of A 100% Renewable Energy Plant For Flexible Local Production Of Electricity, Heating, Cooling, And Fuels, IRENEC2013, 3rd International 100% Renewable Energy Conference, June 2013.

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Paper 7: ISI Journal Paper : Hoffmann, J. Rudra, S.; Rosendahl, L; Toor, SS; Nielsen, JBH., Conceptual Design of an Integrated Hydrothermal Liquefaction and Biogas Plant for Sustainable Bioenergy Production, Bioresource Technology, volume 129, page 402-410.

Paper 8: Journal Paper: Rudra, S.; Kim, HT., A simulation study of Solid Oxide fuel cell for IGCC power generation using Aspen Plus**,** Journal of Energy and Climate Change, Vol. 5, No. 2, 10.2010, p. 24-35.

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"This thesis has been submitted for assessment in partial fulfillment of the PhD degree. The thesis is based on the submitted or published scientific papers which are listed above. Parts of the papers are used directly or indirectly in the extended summary of the thesis. As part of the assessment, co-author statements have been made available to the assessment committee and are also available at the Faculty. The thesis is not in its present form acceptable for open publication but only in limited and closed circulation as copyright may not be ensured.".

to my family

Abstract

This thesis presents the development of a methodology for simulation, techno-economic optimization and design of a quad-generation energy system based on biomass gasification.

An efficient way of reducing CO_2 emission from the environment is by increasing the use of biomass in the energy sector. Different biomass resources are used to generate heat and electricity, to produce gas fuel like bio-SNG (synthetic natural gas) and also to produce liquid fuels, such as ethanol, methanol and biodiesel. Due to the fact that the trend of establishing new and modern plants for handling and processing biomass, it is possible to lay a foundation for future gasification based power plants to produce flexible output such as electricity, heat, chemicals or bio-fuels by improving the flexibility of existing DHP (district heating plant) integrating gasification technology.

The present study investigates energy system alternatives by upgrading existing district heating plant. It provides a generic modeling framework to design flexible energy system for the near future. This framework addresses three main issues arising in the planning and designing of energy systems: a) socio impact at both planning and process design levels; b) technical impact to select different technologies and types of equipment from available options; and c) economic concern to validate new technology with existing ones. To resolve the above issues a life cycle assessment (LCA) analysis and techno-economic analysis of quad-generation systems are included in this study.

The overall aim of this work is to provide a complete assessment of the technical potential of biomass gasification for local heat and power supply in Denmark and replacement of natural gas for the production. This study also finds and defines future areas of research in gasification technology in Denmark within the development of green syngas or liquid fuels for sectors such as the transportation sector. Computational models of whole system component for steady-state operation are developed and also system concepts as well as key performance parameters are identified. The main contribution of this project to ascertain new and flexible technologies that could contribute for local heat demand and supply, national gas grid connection, and short term power marketing perspective in an economic evaluation.

Acknowledgement

The great Bengali poet and Nobel laureate Ravindronath Tagore wrote “It is easy to express the words of knowledge, but the words of feeling are far too difficult”. It is indeed hard form to express my exact feelings of gratefulness to my supervisor Professor Lasse Rosendahl. I am indebted to him for his precious guidance, patience to solve my mistake, and most of all the blue-chip care he has shown towards me, sometimes with righteous suggestions, sometimes with pugnacious words. I also wish him and his dear family a life full of comfort, happiness, and achievements.

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I would like to thank the whole research group at AAU, for so much guidance along the way, and for providing such a friendly atmosphere at work. Sharing my time with such a diverse and skilled group of scientists gave me not only the opportunity to discuss with them about research but also to understand many different characteristics of our cultures and backgrounds.

Special thanks to Kjeld Kærgaard Jensen and Jonas Kromann from Aalborg Kommune for their time to visit some local plants within the work of Fleksenergi.

I would love to thank my all of friends, especially Bangladeshi friends, who helped me a lot to pass a good time during last three years.

On the personal side, my dearest parents would find the most esteemed place in this dissertation and in my heart for their unconditional love, guidance and prayers. All my accomplishments are meaningful if I achieve their satisfaction and likewise worthless without their consent.

Aalborg, April 2013 Souman Rudra

List of publications

This thesis is based on the collection of the papers listed below supplemented by an executive summary. Most of the details of this research study are contained in the attached papers and therefore the present manuscript should be intended only as an outline of the overall project.

The study is the outcome of my work as a PhD student at the Department of Energy Technology, Alborg University, Denmark, from May, 2010 to April, 2013 and spring 2012 at the Department of Mechanical Engineering, University of Alberta, Canada. The work has resulted in five journal papers and three conference papers. The list of the publications is provided below:

Publications:

1. Primary publication:

Paper 1: ISI Journal Paper: Rudra, S.; Rosendahl, L; Blarke MB; Proposal of a biomass based Quadgeneration system for power, heat, cooling and SNG production. International journal of green energy (under review)

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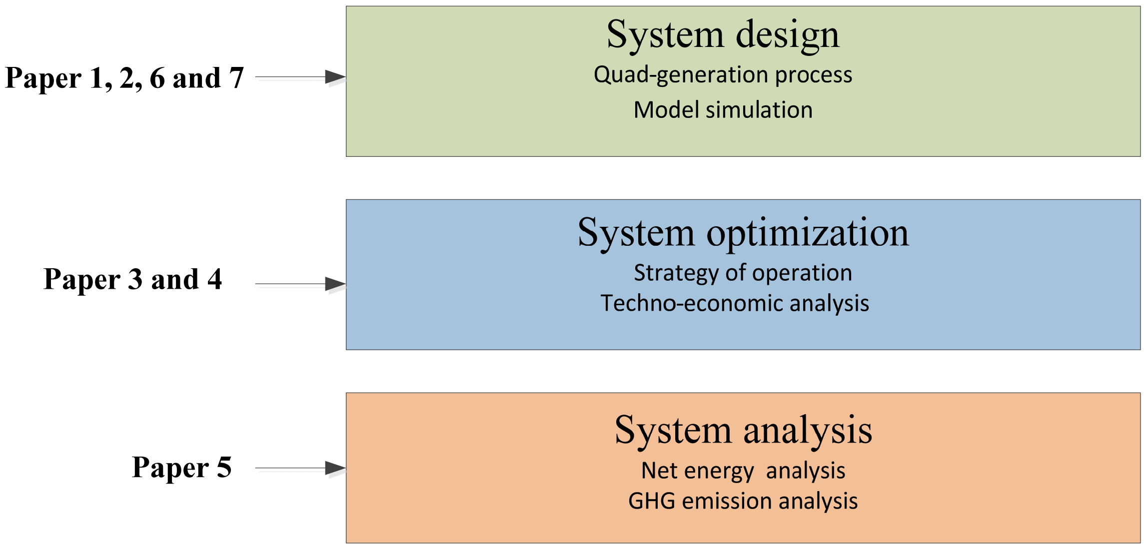

Figure 1: Areas of investigation for each set of papers.

Notes: This thesis includes all the primary papers and secondary papers. As the subject characterized by a broad interdisciplinary perspective, publications have been arranged in three different areas of research as shown in figure.1.

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1

Introduction

Due to high degree of reciprocal relations in social, economic and technological advances, socio-technical energy systems appear in a non-linear custom. So, at the beginning of development it is highly uncertain to justify a new technology in terms of its impression to the society, which kind of factors will become involved, where it could be applied, and which kind of economic models will be applicable. Thus, analysis of technology futures is important for addressing such kinds of questions to inform management as well as policy makers.

The DHS (district heating systems) utilizes the technologies to deliver generated heat from a central location to homes and businesses for space and water heating in Denmark. Some of the DHS are still using fossil fuel as their primary fuel in the North Jutland region. In order to be 100% renewable in future energy system, a quad-generation concept is introduced in this thesis. Quad-generation is the production of power, heat and cooling and different fuels from single feedstock or from flexible feedstocks such as biomass, waste, refinery residue etc. Locally available energy resources are considered and an energy system is designed.

The aim of this thesis is to integrate district heating plant with biomass based gasification plant which can produce different products according to fluctuating energy demand. It also helps to establish an energy network that can help to reduce the heat price difference in different regions. In addition, it presents the concepts for the investment planning of a quad-generation energy system in the North Jutland region, and uses these concepts for different case studies addressing the system for production of power, heat, cooling, gases or liquid fuels.

Quad-generation plant is designed and analyzed thermodynamically by Aspen Plus —a process simulation software. The production plant consists of a gasification step, where the solid fuels are converted to gas at high temperature by adding oxygen or air, gas cleanup steps, CHP (Combined heat and power) and fuel synthesis steps. The gas consisting of CO and H_2 is then used for both gas engine and synthesis unit which convert this gas to bio-SNG (Synthetic Natural Gas) and methanol under high pressure. Then, a distillation step separates the produced products. A gas engine produces both heat and power which can be supplied to the end users. A heat pump is also introduced, which uses the power output from the gas engine and produce both heat and cooling. This heat output can be utilized for district heating, district cooling and also for storage purpose. All the individual systems are simulated by Aspen Plus software. Besides, the thermodynamic analyses, techno-economic analysis of this system are also done with energyPRO software which established this model in the economical point of view. Then, through economical point of view, system analyses are verified with system simulations. A life cycle assessment (LCA) for quad-generation plant is also presented to find the best pathway to produce quad products. These constitute a highly flexible power plant able to run on a number of different fuels and produce electricity, heat, gas, or liquid fuels depending on what is required.

This work emphasizes on the impact of economic and policy circumstances on the optimal design and operation of quad-generation systems. The objective is to maximize the efficiency and techno-economic performance of quad-generation plant while satisfying all design and operational constraints.

1.1 Background

The Danish Government's policy is that Denmark must be a green sustainable society. In Denmark, the description of concrete technological alternatives and the plans for alternative energy play an important role. Denmark plans to be among the top three countries in the world in increasing the share of renewable energy by 2020 ("Energy Policy Statement 2010" 2010).At present the share of renewable energy is coming close to 20 per cent. From such point of departure, The Danish Commission on Climate Change Policy has prepared a report concerning the vision of how Denmark can become independent of fossil fuels and reduce greenhouse gas emissions markedly 2050 (figure 1.1). One of the steps identified for those aims is to optimize the decentralized district heating plant by reducing the fossil fuel uses and introduce locally available renewable resources as the primary fuel for those power plants.

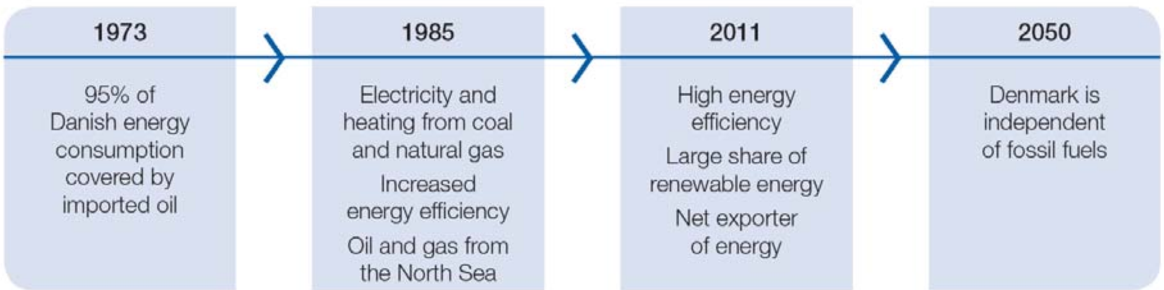

Figure 1.1: Phases in the transition of the Danish energy system("Energy Strategy 2050- from Coal, Oil and Gas to Green Gas" 2011).

In Denmark, district heating covers more than 60% of space heating and water heating. In 2008, 80.5% of this heat was produced by combined heat and power plants. Heat recovered from waste incineration accounted for 20.4% of the total Danish district heat production. Figure 1.2 shows electricity and heat production plants in Denmark. This shows the scenario of central and distributed power plant in Denmark.

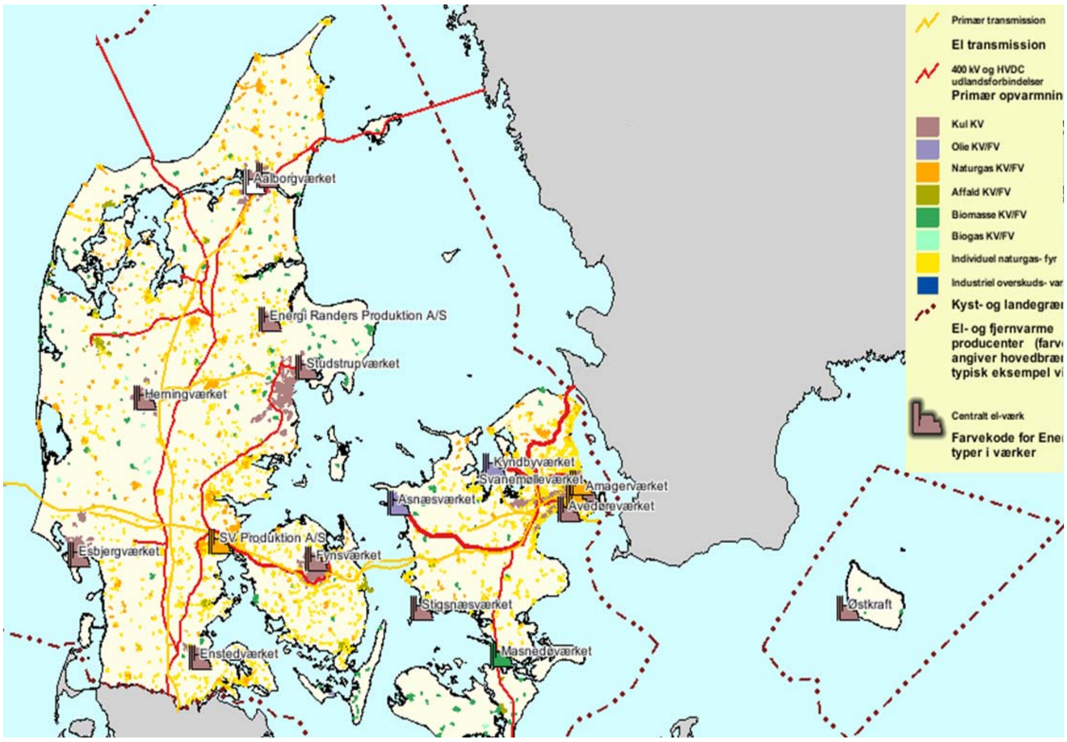

Figure 1.2: Electricity and heat production plants in Denmark, 2010 ("Danish Energy Agency, Ministry of Climate and Energy." 2012).

The Danish District Heating Association represents more than 400 district heating companies in Denmark. These companies supply 98% of the district heating sold in Denmark to more than 1.6 million households ("Danish Energy Agency, Ministry of Climate and Energy." 2013). They are almost all 15-20 MW DH plant. Typically, CHP are either centralized or distributed. Centralized CHP are usually much larger than distributed CHP. 16 centralized and approximately 415 distributed plants supply public heating in Denmark.

According to IEA (International Energy Agency), 13% of the world's total energy use is renewable energy and among the renewable energy resources 77% is bioenergy, where 87% is wood biomass (figure 1.4)

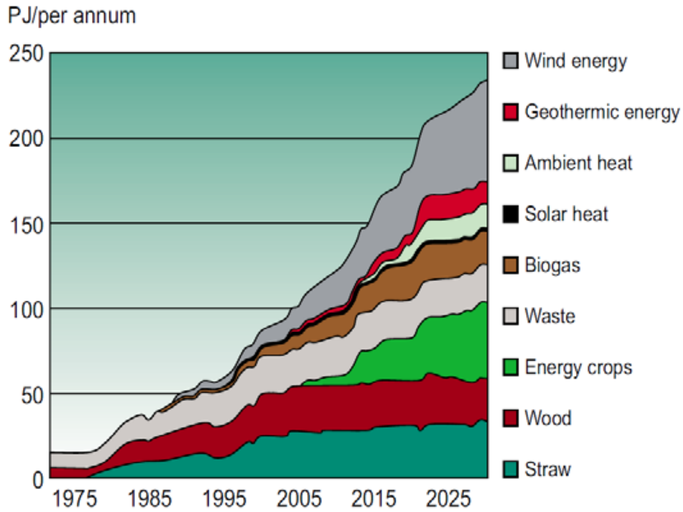

Figure 1.3: Energy 21 proposal for the use of renewable energy sources up to the year 2030 (Skøtt T and Hansen MT, 2000)

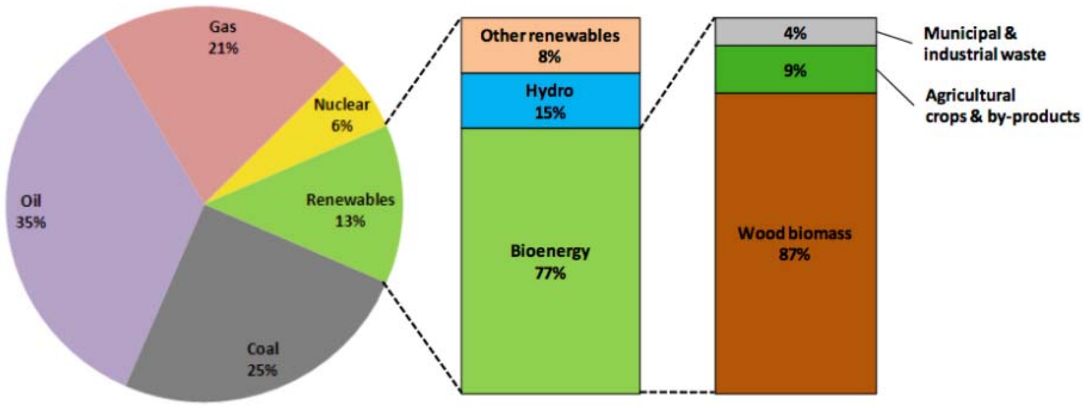

Figure 1.4: Share of Biomass in the world primary energy mix ("Bioenergy- a Sustainable and Reliable Energy Source." 2009).

In Denmark, biomass currently accounts for approximately 70% of renewable-energy consumption, mostly in the form of straw, wood and renewable wastes. The consumption of biomass for electricity and district heating has increased significantly (figure 1.5).

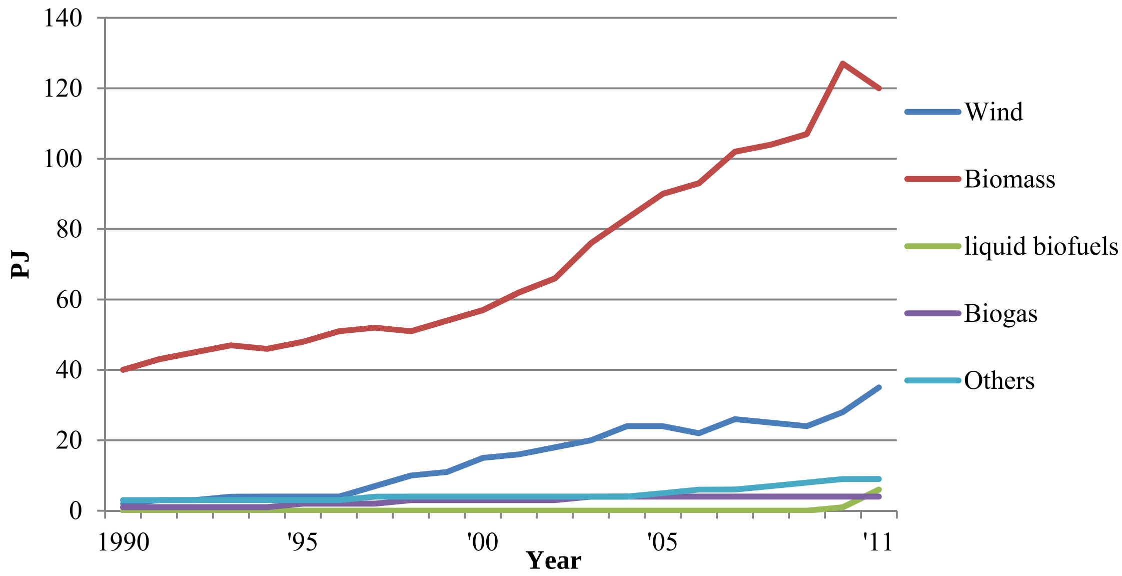

Figure 1.5: Renewable energy consumption by source("Energy Denmark 2011" 2012)

To meet the best utilization of biomass resources and also to decrease the use of fossil fuels in the transportation sector, we have to look for the possible technologies for this quad-generation to produce gaseous/ liquid fuels from local renewable resources. This will make room for more wind mills, wave power and solar energy. It should be ultra-flexible in production and able to run on many different types of fuels. The concern is that, it has to introduce the new technology for producing gas and liquid fuels for the transport sector or for public gas grid. In addition, utility demands in electricity, hot water, cooling and bio-fuels have to be satisfied to meet the end-users needs.

1.2 Motivation

Reviews presented in the previous section shows that significant number of district heating plants are still using fossil fuels, specially natural gas and coal. The present use of the fossil fuels in the DHP represents an increasing environmental and climate-related load. So, investigations have been made to reduce the use of fossil fuels for district heating system and make use of the local renewable resources (biomass, biogas and geothermal) for district heating purpose. Due to environmental and urgent energy situation, this quad-generation approach could be interesting to implement in near future.

The motivation of this thesis is thus to offer a generic framework of methodologies for planning and design of energy systems at different modeling point of views and from different economic views, and demonstrate the quad-generation energy systems for its potential and ability in different applications. There are some other motivations regarding this work which is listed below:

1) High fuel efficiency:

In order to improve the efficiency of local DHP or centralized CHP plant, quad-generation energy system could be appropriate as it diversities both input and output.This technology is expected to have the potential to bring about a dramatic increase in system efficiency, contributing, in the future, to the safeguarding of energy resources.

2) Operational Flexibilities and integration simplicities:

In Denmark, a large amount of electricity is produced by wind energy, but the output varies with the availability of wind. In the cases of excess power production from wind can be utilized to produce H_2 for CH_4 synthesis. Therefore, a quad-generation power plant can be used in conjunction with the wind energy because it has flexible in and output. One of the advantages of this design is that the plant authority does not need to build storage for bio-SNG as they already have access to the national natural gas grid. In this context, this research investigates a process that converts biomass into bio-SNG, which is equal in quality to fossil-derived natural gas. This product can easily be injected into the national gas grid to benefit from the existing distribution network for transport applications.

3) 100 % renewable:

This type of quad-generation sytem offers a valid technological conception for complete 100 % renewable local energy systems that perfectly integrates several processes to supply local energy requirements, even the need for transportation fuels.

1.3 Definition of research questions

- What type of system design may be applied for future energy system and which are the optimal system configurations regarding to fuel processing?
- How quad-generation perform in terms of energy, environment and economy?
- How does this system meet the local heat and cooling demand and also sells competitively electricity and gas to the national grid?
- Can an optimum system operation strategy be identified?
- Some of the district heating plants in Demark are still using fossil fuel energy for their production. How can we reduce the use of fossil fuel and introduce the local renewable fuels for local energy consumption?

1.4 Modeling approach

This thesis evaluates a concept for quad generation by which a combination of electricity (some of which is self-generated) and biomass (here agricultural straw for energy), is converted to produce all four basic energy services: electricity, heat, cooling, and liquid or gaseous fuels. The methodology applied to find the research goal is presented in this section.

- Introduction of quad-generation energy system: A general description of quad-generation has described in chapter 2.
- Conceptual design and modeling for energy system.
- Aspen Plus simulation for individual unit.
- energyPRO simulation for local district heat plant and COMPOSE simulation for entire quad-generation system.
- To find some graphical presentation to validate the newly designed system for the future research development or applications.

1.5 Technology description

Quad-generation energy system consists of different and individual process for power, heat cooling and bio-fuel. As the overall works were published in journals and conferences, the following table 1.1 shows the research steps with in this whole research framework:

Table 1.1: Areas of investigation for research steps (i.e. Data Collection; Core Work; Results; Implications)

	Paper 1 and paper 2	**Paper 3 and 4**	**Paper 5**
Data collection	-Biomass properties -Component modeling	-Danish Heating plant -Energy demand	-Danish Biomass demand, and supply -Feedstock analysis
Core work	-System modeling -Aspen plus simulation	-Simulation in energyPRO -COMPOSE simulation	-Development of net energy ratio -life cycle GHG emission factors
Results	-Part load operations -Quad-generation system configuration -Performance analysis	-Strategic operation -Fuel selection	-Best pathway for quad-generation
Implications	Recommendation for CHP and biomass based gasification plant		

1.6 Literature review

In this section, the aspects about the development of biomass based quad-generation system are described from two prospective. Firstly, an analysis of different studies on biomass process integration with district heat. Secondly, a description of the different modeling approaches on quad-generation energy systems.

1.6.1 Biomass process integration with heating plant

In Denmark, district heating plays a major role in the long term energy scenarios for the future energy system. Today's Danish energy system is characterized by a very diversified and distributed energy generation, based upon three major national grids; these are the power grid, the district heating grid, and, finally, the natural gas grid (Münster et al. 2012). There is a substantial number of biomass-fired district heating plants, approximately 10 straw or wood-chip-fired decentralized combined heat and power (CHP) are also in operation. The rest of the decentralized CHP plants are fuelled by natural gas. More than 15 PJ of biomass and 8 PJ of natural gas are utilized in heating plants, and 30 PJ of natural gas and 18 PJ of biomass are utilized in decentralized CHP plants ("The Danish Energy Agency's Large and Small Scale District Heating Plants" 2013). From this point of departure, (Münster et al. 2012) suggested a scenario framework, in which the Danish system is converted to 100 percent renewable energy sources (RES) by the year 2060, including reductions in space heating demands by 75 percent. In addition, the European Commission developed political strategies to increase the share of renewable and sustainable energy in fulfilling the overall energy demand ("European Commission. Combating Climate Change – the EU Leads the Way"; Hetland, Zheng, and Shisen 2009)

District heating offer both the reduction of the use of fossile fuels and the achievement of higher energy efficiency. To achive these benifits, the best option would be the integration of heat with other production like power, cooling, fuels etc. (Isaksson et al. 2012; Egeskog et al. 2009; Holmgren et al. 2012; Berndes et al. 2010; Wetterlund, Pettersson, and Harvey 2011). To integrate with DH, most significant biomass gasification facilities are presented in this section. Biomass gasification with combined cycle CHP enables a higher power-to-heat ratio than conventional combustion with steam cycle technology, yielding more electricity produced for a given DH demand (Difs et al. 2010). District heating combined with cogeneration has been used for past several years in Northern Europe but it has not been considered as a viable option for areas with warm climate up to now; In eastern Europe areas traditional cogeneration applications tend to prove financially unviable, due to the short operational time within the year(Chinese and Meneghetti 2005).

1.6.2 Quad-generation modeling

A review of the most significant applied biomass gasification facilities for a novel quad-generation system is presented in this section. Much progress is achieved regarding the design of biomass-based polygeneration systems, using simulation technologies. The most stable state-of-the-art gasification technologies in combination with the possibilities of cogeneration through the gasification of biomass are described and compared in a Danish context (Ahrenfeldt et al. 2013), and it showed that the thermal gasification of biomass is both highly flexible and efficient.

The ORC (Organic Ranking Cycle) and gasification for tri-generation technologies for the purposes of serving a specific heating and cooling demand are compared in financial and technological terms (Rentizelas et al. 2009). An ICE (Internal Combustion Engine) is integrated with a downdraft biomass gasifier to supply electricity, hot water for space heating and cold to a commercial building (Huang et al. 2011).

Some articles provide essential information on kinetic mechanisms to describe the conversion during biomass gasification, which is crucial in designing, evaluating and improving gasifiers (Giltrap, McKibbin, and Barnes 2003; Gerber, Behrendt, and Oevermann 2010; Radmanesh, Chaouki, and Guy 2006; Sharma 2008; Roy, Datta, and Chakraborty 2009; Babu, S.P. 2006; Gøbel et al. 2007).

There are a number of scientific publications deal with some novel concepts for polygeneration systems' design and energy analysis — using different input fuels (Qian et al. 2009a; Gao et al. 2008). These articles found that system integration with gasification technology made a significant contribution to the improvement of performance.

The concepts of polygeneration and energy integration are described using various examples of systems (Yu et al. 2010), and the mathematical modeling and simulation of polygeneration energy systems(Li et al. 2010; Wang, Zheng, and Jin 2009a; Paviet, Chazarenc, and Tazerout 2009). So, these articles focus on the evaluation of new plants and technologies concerning the configuration design of the processes. With the aim of achieving higher efficiency and lower emissions, innovations in both power generation technologies and process integration strategies are taken into account in the development of a fully integrated plant (Sadhukhan et al. 2010; Rudra et al. 2010; Djuric Ilic, Dotzauer, and Trygg 2012).

2

Process Design of Quad-generation Energy System

2.1 Energy production from biomass

Biomass is a significant replacement for coal. Conversion from coal to biomass at both central and decentral CHP plants will be made more attractive by allowing producers and consumers to make price agreements. Similarly, the DHPs that are small and struggling with high heating prices can now produce heating based on biomass.

The bulky and inconvenient form of biomass is the main barrier to a rapid shift from fossil fuels to biomass fuels. Unlike gas or liquid, biomass cannot be handled, stored, or transported easily, especially in its use for transportation. This provides a major motivation for conversion of solid biomass to liquid or gaseous fuels, which can be achieved through different pathways (figure 2.1).

2.1.1 Biomass conversion:

Biomass conversion can be divided into three main pathways: thermochemical conversion, physical-chemical conversion and biochemical conversion (Turkenburg W.C. 2000). Figure 2.1 shows the possible biomass conversion. The choice of conversion technique selected for a specific biomass feedstock results in different amounts and forms of useful energy. Biomass can also be refined through mechanical treatments such as extraction (e.g. oil from seeds) or pelletizing. The thermochemical pathway can be further subdivided into combustion, gasification and pyrolysis (R.C. Brown 2004).

Gasification converts the biomass into a gas that can subsequently be used to generate heat and electricity or be converted into fuels or other chemicals (R.C. Brown 2004; Mohan, Pittman, and Steele 2006; Faaij 2006) where pyrolysis converts the biomass into a mixture of char, liquid and gas, and is usually considered as a pre-treatment option for long-distance transportation. The biochemical pathway can be divided into two main paths: digestion and fermentation into methane and ethanol, respectively (Turkenburg W.C. 2000). The conversion of biomass to polygeneration output via gasification and combustion technologies is a renewable technology that can substitute fossil fuels (Steubing, Zah, and Ludwig 2011; Rosendahl LA 2010).

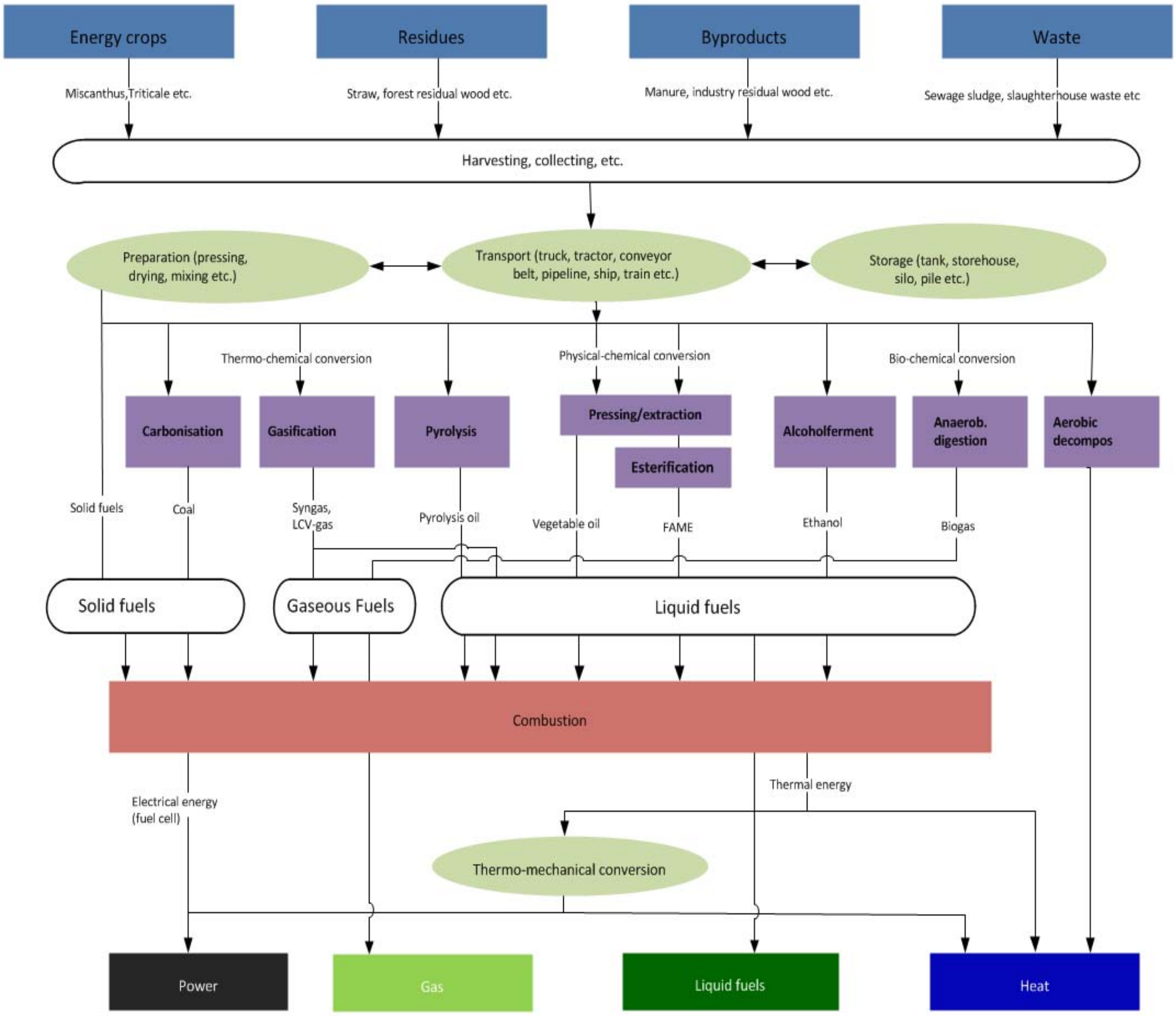

Figure 2.1: Possibilities of energy provision from biomass.

2.1.1 Biomass gasification

Gasification is defined as thermal conversion of organic material to combustible gases under reducing conditions with oxygen added in sub-stoichiometric amounts. Gasification can be accomplished through the direct addition of oxygen, using exothermic oxidation reaction to provide the energy necessary for gasification, or by pyrolysis through addition of sensible heat in the absence of added oxygen.

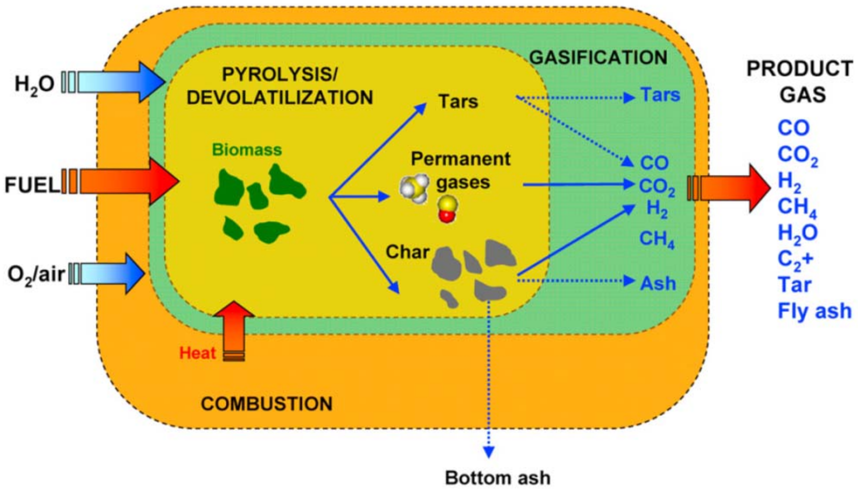

Figure 2.2 : Schematic diagram of gasification processes (Gómez-Barea and Leckner 2010).

Biomass gasification means partial combustion of biomass resulting in production of combustible gases consisting of Carbon monoxide (CO), Hydrogen (H_2) and small amount of Methane (CH_4). This mixture is called producer gas or syngas. Syngas can be used to run internal combustion engines (both compression and spark ignition), as substitute for furnace oil in direct heat applications and to produce SNG (Synthetic Natural Gas) or methanol in an economically viable way. Since any biomass material can undergo gasification, this process is much more attractive than ethanol or biogas production. Figure 2.2 represents the gasification process in a fluidized bed gasifier(Gómez-Barea and Leckner 2010).

2.2 Quad-generation fundamentals

2.2.1 Quad-generation concept:

Quad-generation is the ability to produce of power, heat and cooling and different fuels from flexible feedstocks such as biomass, waste, refinery residue etc. In order to accommodate more renewable energy into the energy system, it is extremely necessary to develop new flexible energy system that can quickly increase or decrease the production of electricity. Such plants should be ultra-flexible in terms of production and able to run on many different types of fuels. In this type of flexible systems (Figure 2.3), the various product rates could change throughout the lifetime of the plant in response to market conditions in different scenarios.

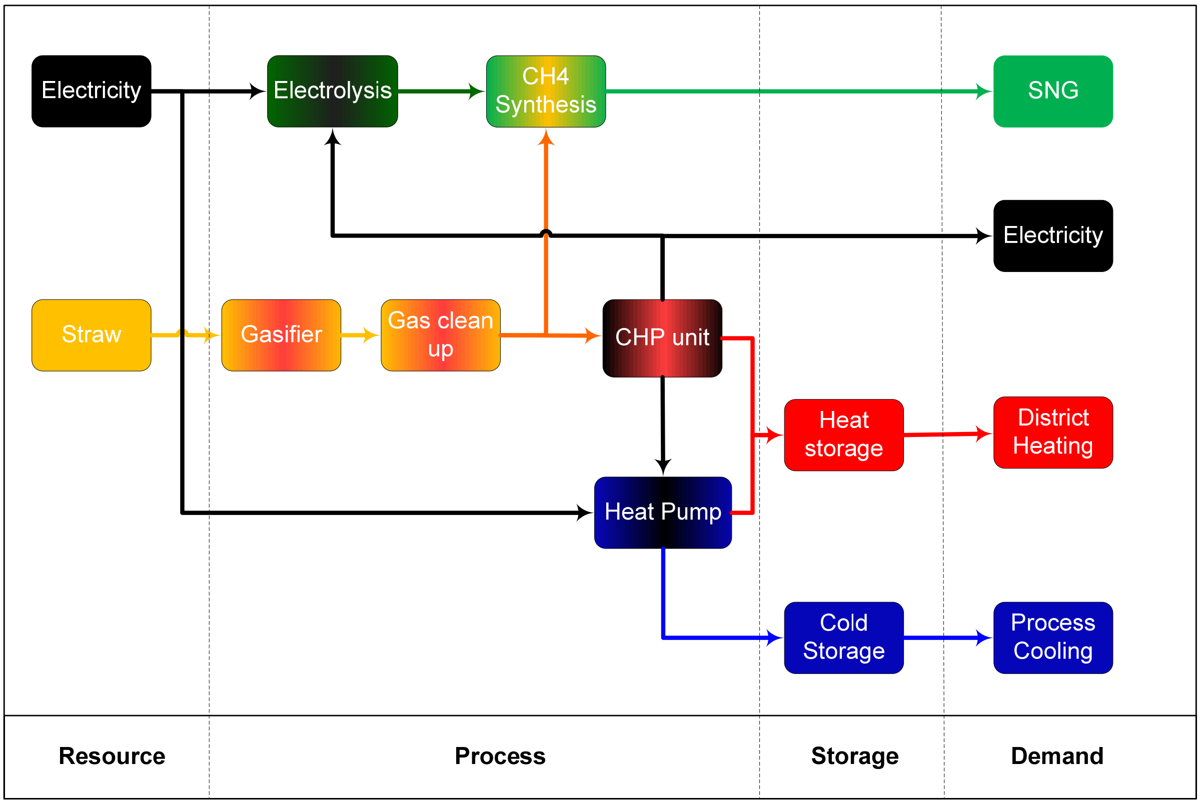

Figure 2.3: Schematic of quad-generation energy system.

2.2.2 The trend of cogeneration to tri-generation, quad-generation and poly generation:

Electricity is commonly produced as a single-output in power plants. Chemical energy of fuel is transformed to electricity with efficiency around 35-40%. The rest of the fuel energy cannot be utilized and it leaves the power plants in the form of waste heat. On the other hand, the heat energy for heating of buildings is commonly produced in boilers with efficiency close to 80 %. When a plant produces both power and heat then it is called co-generation or CHP plant. Low temperature or cooling systems are most frequently produced with utilization of a heat pump driven by electricity. Cooling production signifies a technology with major consumption of energy. When cooling involves a cogeneration plant, it becomes to trigeneration. The increased demand of bio fuel for transportation and other purposes brought the trend of trigeneration, which led towards quad-generation — where power, heat, cooling and biofuel can be produced form single input. Quad-generation in energy systems also utilizes the waste heat, released during the generation of electricity from power plant. So, Quad-generation significantly increases efficiency by increasing utilization of primary energy sources. Thus, the concept of quad-generation characterizes efficient production of energy for effective local energy consumption. The short-distance connection between the location of generation and the location of consumption is an important advantage that allows the action of the majority of the generated energy.

The character of locally distributed energy systems evolves from co-generation systems (electricity and heating), over tri-generation systems (electricity, heating, and cooling), to quad-generation systems (electricity, heating, cooling, and liquid or gaseous fuels). Thereby, a single integrated state-of-the-art distributed energy plant may come to provide for all local energy residential, commercial, industrial energy demands, including transportation fuels.

2.2.3 System description and design

A quad-generation system is proposed, as illustrated by the flowsheet in figure 2.4. The process is described by the following steps:

1. The biomass is gasified in the presence of air at atmospheric pressure.

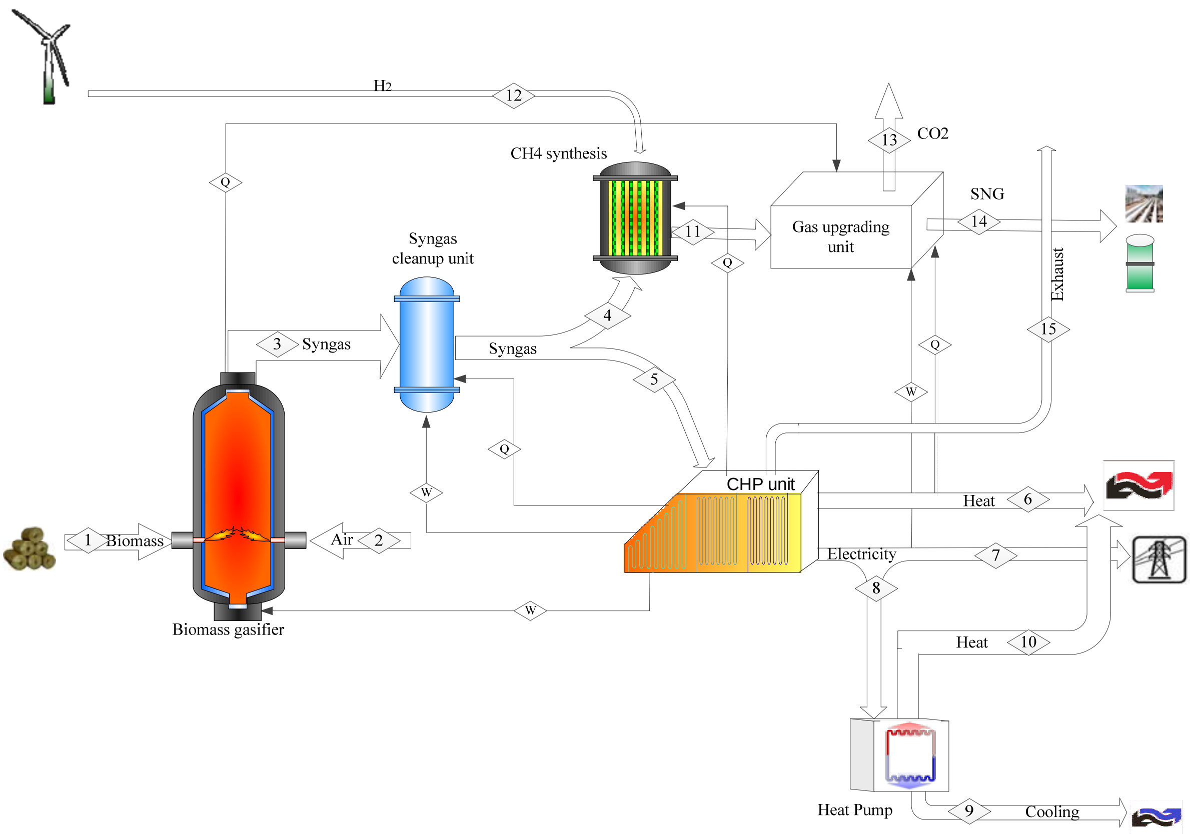

Figure 2.4: Schematic of the proposed quad-generation system.

2. The syngas leaving the gasifier will be cooled and cleaned by a gas cleanup unit. The particulate matter is removed from the raw syngas, exiting the gasifier, using a cyclone collector and a candle filter system.

3. One of the streams from the syngas cleanup unit will be sent to the engine for power and heat production, while a compression heat pump is introduced. It is a flexible compressor-driven unit — able to produce both cooling and heating.

4. The synthesis gas can contain a considerable amount of methane and other light hydrocarbons, representing a significant part of the heating value of the gas. Therefore, another stream from the gas clean-up section enters the CH_4 synthesis section to be converted to CO and H_2 driven by the addition of steam over a catalyst at high temperatures. Subsequently, it maintains a proper H_2: CO ratio for methane synthesis. In the water-gas shift reaction, CO and H_2O are converted to CO_2 and H_2.

5. In the methanation reactor, CO and H_2 are converted to CH_4 and H_2O in a fixed-bed catalytic reactor. Since methanation is a highly exothermic reaction the increase in temperature is controlled by recycling the product gas or using a series of reactors. After gas upgrading, bio-SNG is ready for applications.

The transformation of raw materials of the desired chemical products usually cannot be achieved in a single step. Instead of the overall transformation is broken down into a number of steps that provide intermediate transformations. These steps are carried out through reactions, separation, mixing, heating, changing cooling pressure, and changing size (both reduction and enlargement). The process involved two broad activities. Firstly, individual transformation steps are selected. Secondly, these individual transformations are interconnected to form a complete process.

Table 2.1: Biomass characteristics **(**DM: dry matter; DAF:dry ash free**)**

Properties /Biomass		Straw	Wood chips
LHV (MJ/kg)		17.65	16.8
Ultimate Analysis	C	43.65	63.04
(wt%)	H	5.56	5.11
	O	43.31	29.41
	N	0.61	0.24
	S	0.01	0.52
	Cl	0.6	0
	Ash	6.26	1.68
	VM	75.17	40.08
Proximate Analysis (wt%)	FC	19.25	38.58
	Ash	5.58	1.34

2.3 Process analysis

This section describes the different process of quad-generation plant model. The subsections elaborate the steps, from pretreatment of biomass to end products.

2.3.1 Pretreatment of biomass

Fuel analysis indicate that the treated biomass (table 2.1) has lower ash content, improved heating value, higher ash deformation temperatures, and higher volatile matter to fixed carbon ratios, than the untreated material (Kumar et al. 2009).

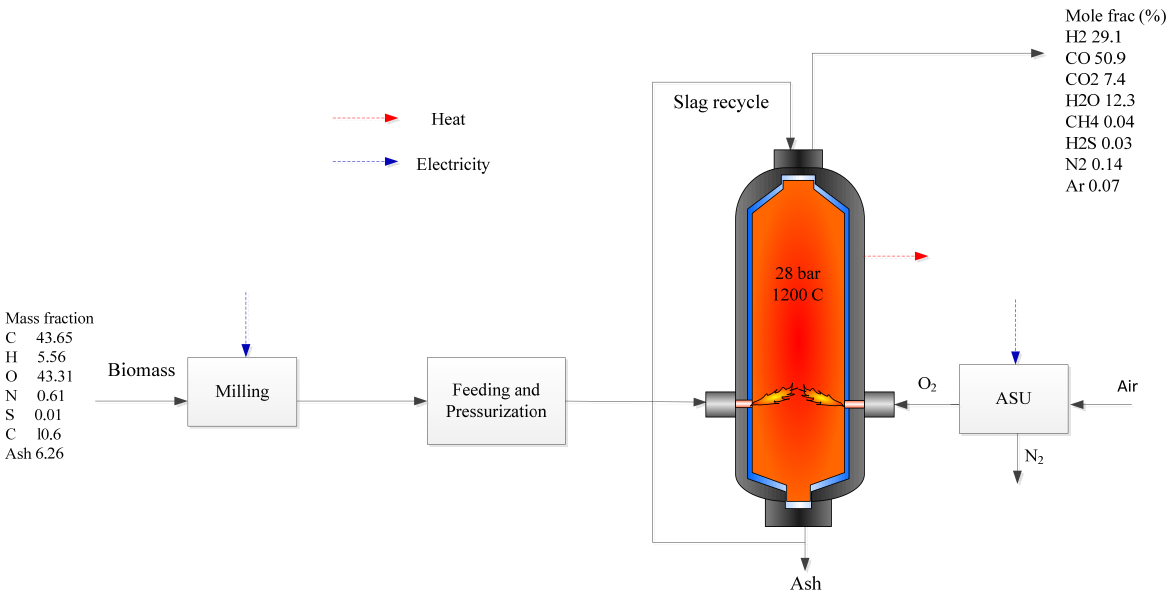

Figure 2.5: Flow sheet of the modeled gasification part, including heat outputs and electricity inputs.

2.3.2 Gasification of biomass

Figure 2.5 shows the modeled gasification process integrating heat outputs and electricity intputs. A typical gasification process generally follows preheating and drying, pyrolysis, char gasification, and combustion steps. In a process, biomass is first heated and then it undergoes through thermal degradation or pyrolysis. The products of pyrolysis react among themselves and with the gasification medium to form the final gasification product (figure 2.6).

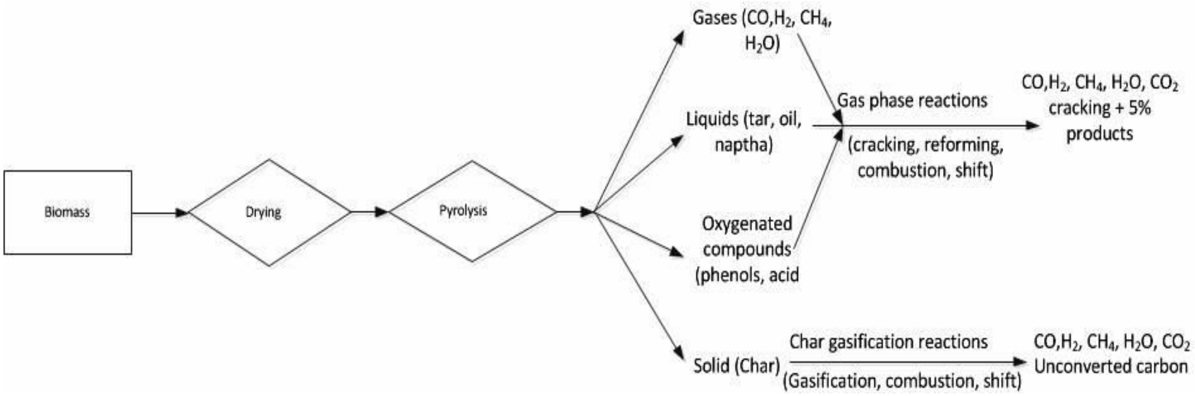

Figure 2.6: potential paths of gasification(Basu, P., 2010)

Gasifying Mediums

Gasifying agents react with solid carbon and heavier hydrocarbons to convert them into low-molecular- weight gas like CO and H_2. The main gasifying agents (table 2.2) used for gasification are;

1. Oxygen
2. Steam
3. Air

Oxygen is a popular gasifying agent, though it is primarily used for combustion process. A ternary diagram (figure 2.7) of carbon, hydrogen and oxygen demonstrates the combustion paths of the formation of different products in a gasifier.

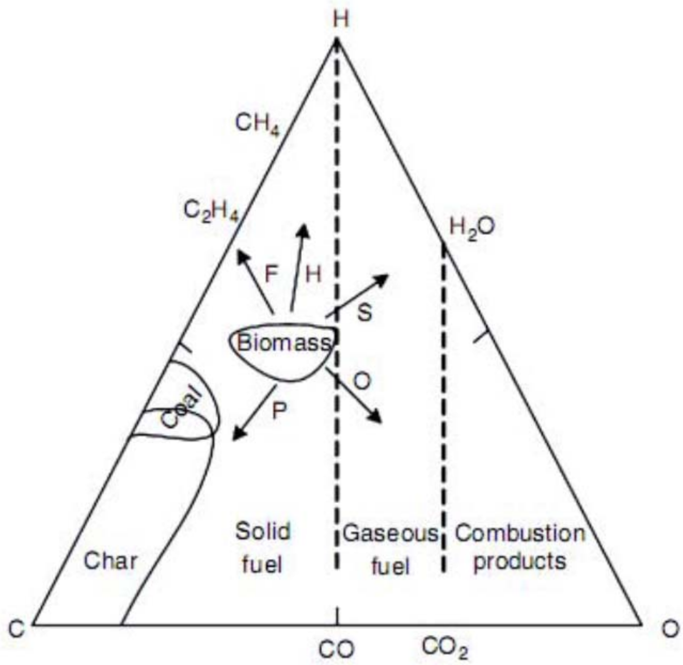

Figure 2.7: C-H-O diagram of the gasification process (Basu, P., 2010)

Table 2.2: Heating values for syngas based on gasifying medium.

Medium	Heating value
Air	4-7
Steam	10-18
oxygen	12-28

The diagram (figure 2.7) is a tool to represent the biomass conversion processes. The three corners of the triangle characterize pure C, O, H- that is, 100% concentration. Points inside the triangle represent mixtures of these three substances. The side opposite to a corner with a pure component (C, O, or H) represents zero concentration of that component.

- If oxygen is used as the gasifying agent, the conversion path moves toward oxygen corner. It produce CO for low oxygen and CO_2 for high oxygen
- If Steam is used as the gasifying agent, the conversion path moves toward hydrogen corner in figure 2.7. Then syngas contains more H_2 per unit of carbon, resulting higher H/C ratio.
- If air is used as the gasifying agent, the nitrogen in it greatly dilutes in the product. The choice of gasifying agent affects the heating value of syngas.

A biomass fuel is closer to the hydrogen and oxygen corners compared to coal. This means that biomass contains more hydrogen and more oxygen than coal contains. Lignin would generally have lower oxygen and higher carbon compared to cellulose or hemicellulose.

2.3.2.2 Chemical reactions during gasification

The gasification involves chemical reactions among the hydrocarbon in fuel, steam, carbon dioxide, oxygen, and hydrogen as well as chemical reaction among the evolved gases. The important chemical reactions taking place in the gasifier can be encapsulated as:

$$C + 0.5O_2 \longrightarrow CO \quad (2.1)$$

$$C + CO_2 \longrightarrow 2CO \quad (2.2)$$

$$C + H_2O \longrightarrow CO + H_2 \quad (2.3)$$

$$C + 2H_2 \longrightarrow CH_4 \quad (2.4)$$

$$CO + 0.5O_2 \longrightarrow CO_2 \quad (2.5)$$

$$H_2 + 0.5O_2 \longrightarrow H_2O \quad (2.6)$$

$$CO + H_2O \longrightarrow CO_2 + H_2 \quad (2.7)$$

$$CH_4 + H_2O \longrightarrow CO + 3H_2 \quad (2.8)$$

$$H_2 + S \longrightarrow H_2S \quad (2.9)$$

$$0.5N_2 + 1.5H_2 \longrightarrow NH_3 \quad (2.10)$$

2.3.3 Gas cleaning process

Syngas from biomass can be simillar with conventional syngas (from coal). Conventional syngas cleaning includes:

- Particle removal by a filter and perhaps a cyclone.
- A Rectisol unit to remove bulk impurities and CO_2
- Guard beds (ZnO and active carbon filters) to remove trace impurities(A. van der Drift and H. Boerrigter 2006)

The syngas from the gasification process mostly consists of CO_2, H_2, CO, CH_4 and water vapor. But, for the existence of trace components in that stream, it is necessary to have numerous gas cleaning steps for synthesizing syngas. The ingredients exiting in the syngas also needs a treatment of particulate matter (ash, bed particles), tars and higher hydrocarbons, alkali metals, as well as sulphur and nitrogen compounds. There are some procedures to remove particulates from the syngas by cyclones, fabricfilters, or by scrubbing separators. Tar content reduce by particle separation from syngas and the extent of such removal is dependent on the separation technology applied (Devi, Ptasinski, and Janssen 2003; Han and Kim 2008). To avoid excessive fouling of the heat exchanger equipment, it is very essential to remove tar from syngas. By using catalytic bed material, it is possible to reduce tar formation during the gasification process (Pfeifer, Rauch, and Hofbauer 2004).

Raw syngas first passes a scrubber to remove particulates and chlorides, and then enters a COS hydrolysis reactor, where almost all COS is converted to $CO_2$and H_2S by the following reaction:

$$COS + H_2O = CO_2 + H_2S \qquad (2.11)$$

The syngas exiting the COS hydrolysis reactor is cooled and passed through a carbon bed to remove over 95% of mercury. Then, cool syngas enters a Selexol unit, where almost all H_2S is removed. The H2S rich stream is sent to the Claus plant, where H_2S is converted to elemental sulfur, a product of the polygeneration process, via the following reaction:

$$H_2S + 0.5\ O_2 = H_2O + S \qquad (2.12)$$

The syngas exiting the COS hydrolysis reactor is cooled and passes through a carbon bed to remove over 95% of mercury. Then, cool syngas enters a selexol unit, where almost all H_2S is removed. The H_2S rich stream is sent to the Claus plant, where H_2S is converted to elemental sulfur, a product of the quad-generation process, via the following reaction:

$$H_2S + 0.5\ O_2 = H_2O + S \qquad (2.13)$$

Alkali traces from the syngas can be removed by both washing techniques and techniques based on solid sorbents. Last one is operated at high temperatures. It is either based on chemisorption or physical adsorption (Turn S. Q 1998). After removing all the impurities, it is ready for using in gas engine and gas synthesis unit.

2.3.4 Heat and Power Process

The syngas from gas cleanup process enter to gas engine and the syngas is then combusted with air in a gas engine to produce heat and power generation. In large-scale systems using gas turbines, the exhaust gas from the gas turbine can be used to raise steam in a heat recovery steam generator to generate additional electricity using a steam turbine (Rankine cycle), resulting in combined cycle operation (Rudra et al. 2010). In a combined heat and power plant, designed for district heating(Bianchi, De Pascale, and Melino 2013), the flue gas from the combustion of the product gas goes through a heat exchange system to raise the temperature of a heat transport fluid, generally water, circulating in a district heating system. Residual heat in the flue gas can be used to dry the biomass prior to its discharge to the atmosphere.

2.3.5 Cooling Process

The quad-generation concept combines straw-fuelled gasification, syngas-fuelled engine and methane synthesis, compression heat pump. A concept for integrating a compression HP (Heat Pump) unit that utilizes heat recovered from the CHP unit(Blarke and Dotzauer 2011a). Large-scale Heat pumps are very efficient heating and cooling systems and can significantly reduce energy costs(Weber et al. 2006). Electricity both from plant and grid can utilize to produce cooling in this quad-concept. A heat-pump can meet the cooling, respectively the heating loads. The availability of a low-temperature heat source or a cooling demand in specific locations may still allow for the addition of such external heat sources, which may then allow for the integration of a relatively larger heat pump.

Heating loads as well as the electricity requirements are obtained from local demand. But cooling demands assume which is listed in paper 4(Blarke, MB, Rudra, S, and Rosendahl, LA 2013). According to this operating mode, both the CHP system and the heat pump supply thermal and cooling to the final user. Depending on the different case, cooling demand covered the compression heat pump.

2.3.6 Bio-SNG Process

Substituting part of natural gas by a Synthetic Natural Gas (SNG) or Substitute Natural Gas is produced from a sustainable primary energy source, with the same properties as natural gas. SNG from gasified biomass is one promising option to produce renewable transport fuels. The production of synthetic natural gas from gasified biomass is one of the alternative pathways for the reduction of anthropogenic greenhouse gas (GHG) emissions. SNG produced from renewable resources results in reduced emissions of CO_2 when replacing fossil natural gas in conventional applications. R&D program of SNG from coal is conducted by ExxonMobile during 1970.

The equilibrium methane yields for the SNG process as a function of temperature and pressure are shown in figure 2.8 (Robert C. Brown 2011).

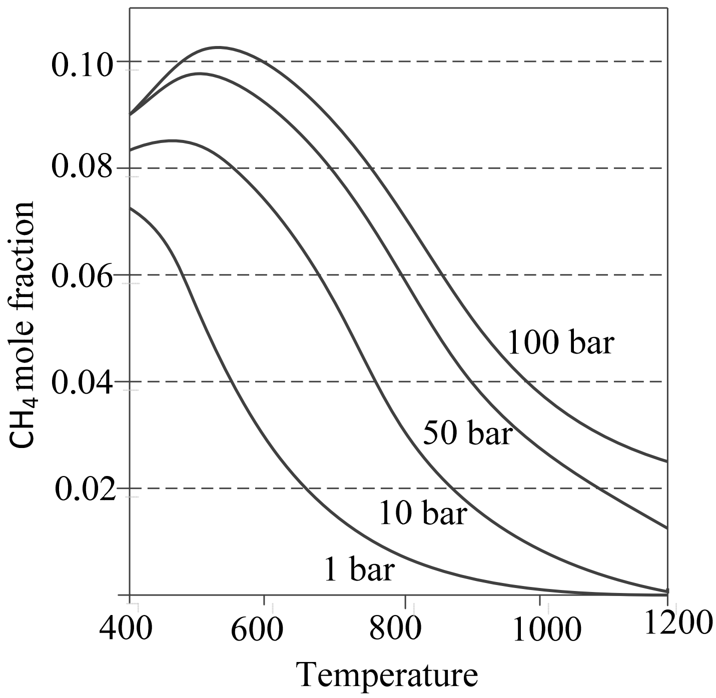

Figure 2.8: Equilibrium methane yields for the SNG process as a function of temperature and pressure(Robert C. Brown 2011).

2.3.6.1 Bio-SNG as a reneable fuel

Replacing portion of natural gas by a bio-SNG produced from renewable primary energy source like biomass, having the same properties as natural gas makes the application of sustainable energy easy as natural gas grids are widely spread in Denmark and in many other countries. Bio-SNG is produced by gasification of lingo-cellulosic materials (e.g. forestry residues, energy crops). The bio-SNG potential is estimated based on the known technologies and the estimated biomass potential for 2020. It is assumed that woody and herbaceous biomass can be converted trough gasification; the anaerobic digestion of wet biomass is also included. Under the given conditions, it is estimated that a potential around 100 PJ of bio-SNG will be available in 2020, including only Danish feedstock (Ahrenfeldt, Jesper, Jørgensen, Betina, and Thomsen, Tobias 2010).

2.4 Modeling tools

Modeling refers to expressing a number of equations that describe mathematically a process under consideration. In simulation, the formulated model is solved by using appropriate solution procedure, as well as by entering the values of independent process variables. Aspen Plus is used for modeling the quad-generation system. Aspen Plus is a component-based thermodynamic modeling and simulation tool. Aspen Plus V7.3 version is used in the modeling. This process simulator is equipped with a large property data bank, containing the various stream properties required to model the material streams in a gasification plant, with an allowance for the addition of in-house property data. Here, more sophisticated block abilities are required; such blocks can be developed as FORTRAN subroutines. It offers a variety of thermodynamic property methods for process simulations. Some investigations conducted on biomass gasification (Wang, Zheng, and Jin 2009b; Doherty, Reynolds, and Kennedy 2010; Nikoo and Mahinpey 2008) showed that Aspen Plus is capable of predicting performance under diverse operating conditions. The Peng Robinson equation of state with the Boston-Mathias alpha function (PR-BM) is used to estimate all of the physical properties of the conventional components in the gasification process ("ASPEN Technology, Getting Started Building and Running a Process Model, Burlington."; Ramzan 2011). These property methods are recommended for hydrocarbon processing applications. The alpha parameter in this property package is a temperature dependent variable that improves the correlation of the pure component vapor pressure at very high temperatures. For this reason, the property package is suitable for simulating gasification processes that involve fairly high temperatures. 'HCOALGEN' and 'DCOALIGT' are selected for the enthalpy and density property models, respectively, for both biomass and ash.

The equation for the Peng-Robinson model as used in the PR-BM property method is:

$$P = \frac{RT}{V_m - b} - \frac{a}{V_m(V_m + b) + bV_m - b} \tag{2.1}$$

Where.

P = Pressure

V = volume

R = Ideal gas constant

T = Temperature

$V = V_m - c$

Where: Vm = Molar volume calculation by the equation of state without the correction/

$c = \sum_i x_i c_i$

(the Peneloux volume correction term) $c_i = 0.50032[\frac{RT_{ci}}{P_{ci}}](0.25969 - z_{RAi})$

Table 2.3: Process design parameter assumptions for simulation.

Item	Unit	Value
Gasification unit		
Temperature	°C	1100
Pressure	bar	25
Air for gasification	t/h	96
Gas cleanup unit		
CO_2 removal	%	95
Sulphur removal	%	95
Electricity (Lv et al. 2004)	kJ/mol (CO_2 + H_2S)	1.9
Steam (Lv et al. 2004)	kg/mol (CO_2 + H_2S)	6.97
Power, heat and cooling unit		
Gas engine inlet temperature	°C	650
Gas engine inlet pressure	°C	25
Air for gas engine	t/h	100
Isentropic efficiency of expanders	%	90
Isentropic efficiency of main compressors	%	88
Mechanical efficiency main compressor	%	98
recycled water for heating	kg/h	2000
recycled water for cooling	kg/h	1000
SNG synthesis unit		
SNG synthesis temperature	°C	270
SNG synthesis pressure	bar	20

The definition of the input data for the calculations was acquired from literature. Regarding the process simulation, the following assumptions have been made:

- The process is steady state and isothermal.

- This process is defined to occur instantaneously at equilibrium with volatile products mostly made of H_2, CO, CO_2, H_2O, CH_4, and C_2H_4 (Lv et al. 2004; Gomez-Barea and Leckner 2010).

- The electricity and steam for gas cleanup unit is extracted from gas engine (CHP unit)

The process design parameter assumptions for the simulation are summarized in Table 2.3. The overall process is divided into different sections, which are described below.

2.4.1 Biomass Drying:

Biomass is specified as a non-conventional component in Aspen Plus and is defined in the simulation model using the ultimate and proximate analysis. Part of the moisture portion of the non-conventional component representing the biomass materials in Aspen Plus is converted to conventional liquid H_2O in a stoichiometric reaction (RSTOIC) block. The proximate and ultimate analysis using Aspen Plus simulation can be found in table 2.1. Air (1.01 bar, 60°C, 50 % relative humidity) is pumped into the dryer. The water is evaporated in a countercurrent heat exchanger block using the process steam as a heat source. A small heat loss is modeled in the condensate return line and is assumed to be 2 % of the dryer thermal load. A FLASH2 block is used to separate the exhaust vapors from the biomass material, and dried product (DRYBIOM) exits the dryer with 10 % moisture content.

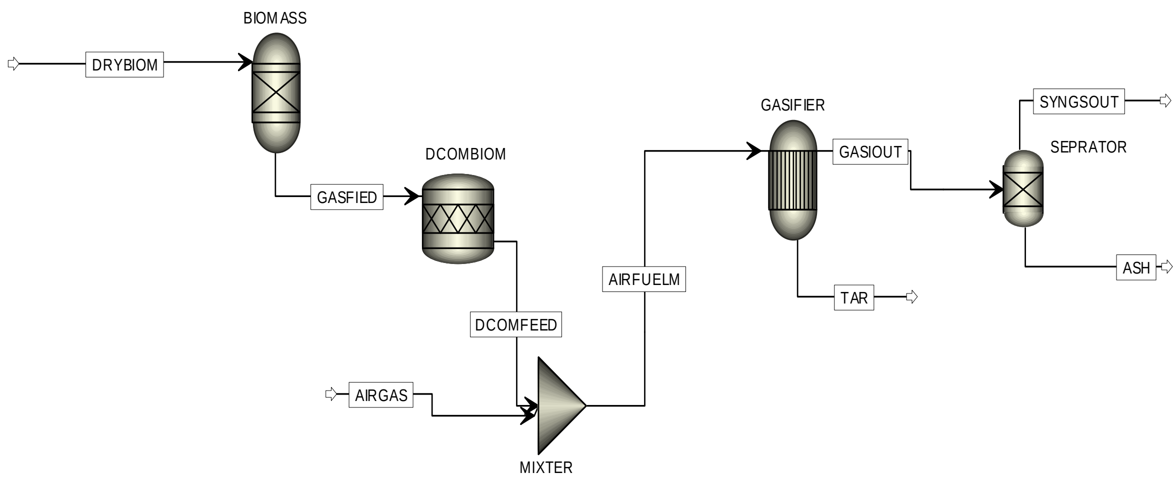

Figure 2.9: Process flowsheet for gasification unit

2.4.2 Gasification Unit:

Figure 2.9 (a) shows processes diagram for gasification unit. 'DRYBIOM' from the drying unit enters the 'BIOMASS' block at near-atmospheric pressure and the component yield of this block has to specify. It moves through an equilibrium reactor 'DCOMBIOM' and mix of air in a 'MIXTER'. The stream continues to a RGIBBS block. It separates tar components from the stream. A description of the different Aspen Plus reactor blocks and process flowsheets are given in appendix table A-1. The gasification reactions occur in ('DCOMBIOM') according to the reaction set given in Eq. (2.1) - (2.10).

2.4.3 Gas cleanup unit:

After the synthesis gas leaves the gasifier, it must be processed for further use. First, the synthesis gas passes through a gas cooling heat exchanger block, 'SYN-HTX', which generates process steam. The gasification of these biomass fuels then produce components such as H_2S and NH_3, which can be harmful to equipment and produce pollutants during synthesis gas combustion. Next, the gas passes through a wet scrubber, 'H2SABS', to remove sulfur matter. After that the stream continues to block 'CO2ABS' where it can produce 'CO2RICH' stream and CO_2 is separated through block 'B1'. The next stage in gas processing is the selective removal of harmful components through 'N2STRP' block. The flowsheet for this gas cleanup unit presented in appendix figure A-1 (b).

2.4.4 Power, heat and cooling production unit:

Clean syngas from the gas clean-up section enters the gas engine, where it combusts in 'COMBA' (figure A-1 (c)). The stream continues into an expander ('EXPN1') and burns in a reactor ('BURN') in the presence of air. The flue gas is used to run 'EXPN2' and 'EXPN3'. The total work from all the 'EXPN's are combined in 'WORKMIX' and are split again into two streams, with 20 % of the produced power used for the cooling system. It is assumed that the split ratio is 80:20. The exhaust gas from 'EXPN3' is used for district heating purposes. District heating water from the users (make-up water) returns as 'DHWIN1' and 'DHWIN2' and is heated by heat exchangers ('B3' and 'B2'). Both 'DHWOUT1'and 'DHWOUT2'outputs from the heat exchangers are utilized for the district heating system.

2.4.5 Bio-SNG production unit:

The 'SYNGASOT' stream leaves the gas cleanup mix with additional hydrogen 'H2IN' in the 'MIXTER' block and continues to the methanation reactor, 'METHANT'. Additional H_2 feed is necessary to provide CO/H_2 ratio. Flowsheet of CH_4 synthesis process presents in appendix figure A-1 (d). In the methanation reactor, CO and H_2 are converted to CH_4 and H_2O in a fixed-bed catalytic reactor.

$$CO + 3\ H_2 \longrightarrow H_2O + CH_4 \qquad (2.13)$$

The produced CH_4 still has some impurities, so it enters a separator unit, 'CO2REMOV', where the CH_4 is separated from CO_2.

Case study:

As the heat demand varies during the year, there is a need for different case studies for the best utilization of total capacity. Therefore, the above system is designed for five cases based on syngas distribution to gas engine and gas synthesis unit. This is discussed in paper no.1 (Rudra, S, Rosendahl LA, and Blarke, MB 2012).

Table 2.4: Different cases based on syngas distribution

	Case name	Power	Heat	Cooling	SNG
Case 1	SNG-0	25	50	25	0
Case 2	QUAD-70	20	35	15	30
case 3	QUAD-50	15	25	10	50
case 4	QUAD-30	10	15	5	70
case 5	SNG-100	0	0	0	100

2.5 Results

The results from process simulation of quad-generation plant are presented in this section. The detail flowsheet of this quad-generation plant is presented in figure 2.9 in modeling tools section and in appendix figure A-1. All the assumptions regarding this quad-generation system are summarized in table 2.3. Table A-2 and table A-3 in appendix represent the steam compositions of gasification unit and syngas cleanup unit respectively. Figure 2.10 (A) and (B) show the simulation results of syngas composition in gasification various with temperature range 800 – 1300 °C.

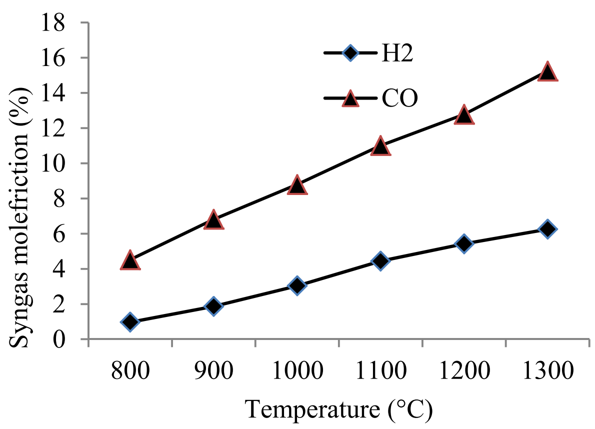

Figure 2.10 (A): Effect of temperature in syngas (H2 and CO).

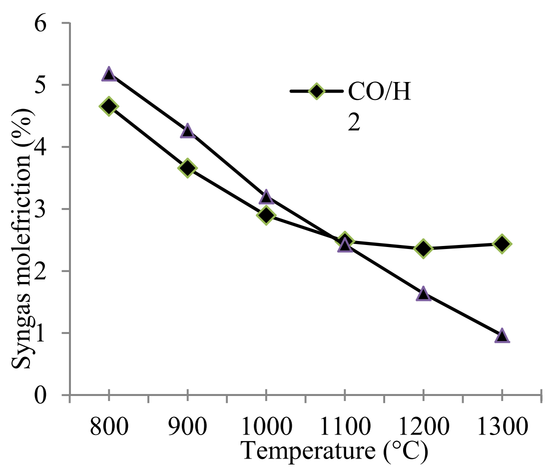

Figure 2.10 (B): Effect of temperature on CO/H2 ratio and CH4

Results on case studies:

The detailed energy consumptions for a quad-generation plant are shown in table 2.5 (based on the description of previous section and table 2.4). For 100 tons per day of dry biomass input, SNG-0 utilizes 7625 kg/h syngas for power, heat and cooling production, while QUAD-25 uses 2287.5 kg/h for power, heat, and cooling production and 5337.5 kg/h for SNG production. The total analysis is published in paper 1.

Table 2.5: The material balance, power, heat, cooling and SNG produced, and utilities of five cases

Items	Units	SNG-100	QUAD-75	QUAD-50	QUAD-25	QUAD-0
Feed stocks						
Biomass	t/day	100	100	100	100	100
Syngas for Power, heat and cooling	kg/h	7625	5718.75	3812.5	1906.25	0
Syngas for SNG	kg/h	0	1906.25	3812.5	5718.75	7625
Air for gasification	t/h	96	96	96	96	96
Air for gas engine	t/h	100	80	60	40	0
Make up water	t/h	3	3	3	3	3
H_2 input	kg/h	0	36.76	42.231	52.41288	66.241
Waste Product						
Ash	Kg/h	138	138	138	138	138
CO_2 capture during gas cleanup	Kg/h	326.98	326.98	326.98	326.98	326.98
CO_2 capture during SNG production	Kg/h	0	131.78	156.23	182.565	204.682

The primary measure of energy efficiency for a power plant is the feedstock to net power production ratio, but because the waste heat generated in the quad-generation plant is used for heat production, cooling, and bio-SNG production.

The equations for efficiency measurement are described in paper 1 (Rudra, S, Rosendahl LA, and Blarke, MB 2012). Figure 2.11 shows that the power efficiency for SNG-0 is 22.5 %, while the efficiency for QUAD-25 is 6.9 %, which is relatively low as it uses less syngas for power production. In the case of heat utilization, heat production efficiency is higher than other output efficiencies. The heat production efficiencies are 24.47 %, 29.37 %, 42.1 % and 54.34 % for QUAD-25, QUAD-50, QUAD-75 and SNG-0, respectively. Figure 2.11 also shows the cooling efficiency, which is the least efficient for all the cases, as it produces a smaller proportion of cooling relative to the total output. For SNG production, the efficiency increases gradually from QUAD-75 to SNG-100.

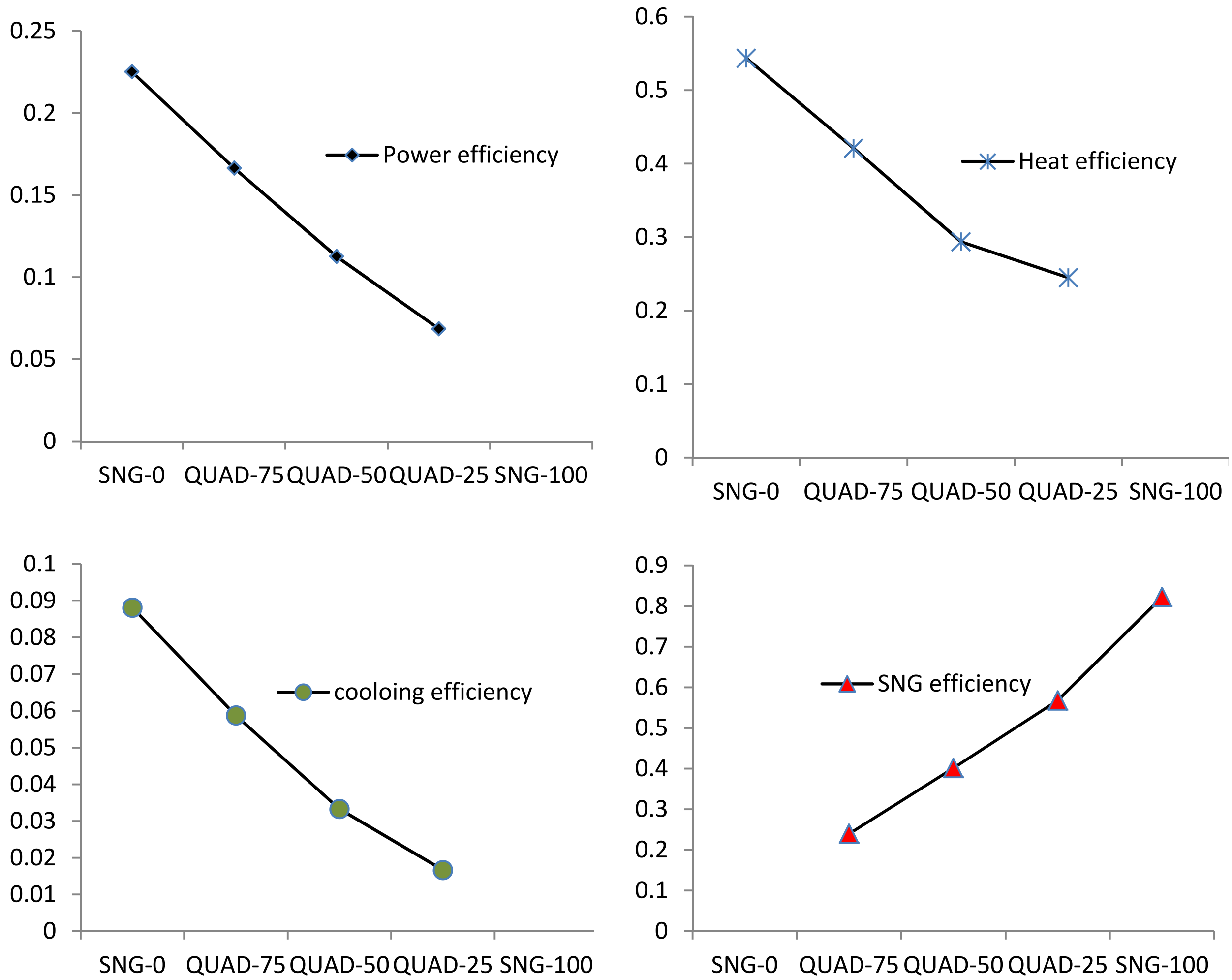

Figure 2.11: efficiency comparison graph for SNG-0, QUAD-75, QUAD-75, QUAD-75 and SNG-0.

An energy balance for the quad-generation system was done for these case studies which was published in paper 1(Rudra, S, Rosendahl LA, and Blarke, MB 2012). Figure 2.12 indicates the amounts of the four outputs from the QUAD-50 case which represent all the four outputs. The sankey diagram for other cases are represented in appendis(figure A-2). It should be noted that the amount of syngas produced from the gasifier has been kept constant for all of the cases (Figure 2.12). According to the different amounts of syngas utilization, this process produces approximately 49.728, 73.595, 95.22 and 134.34 m^3/h of bio-SNG for the QUAD-75, QUAD-50, QUAD-25and SNG-100 cases, respectively. Simultaneously, it generates 11.1, 8.6, 6 and 5 MW of heat in the SNG-0, QUAD-75, QUAD-50 and QUAD-25 cases, respectively. Twenty percent of the power generation from the quad-generation plant is used for the cooling system.

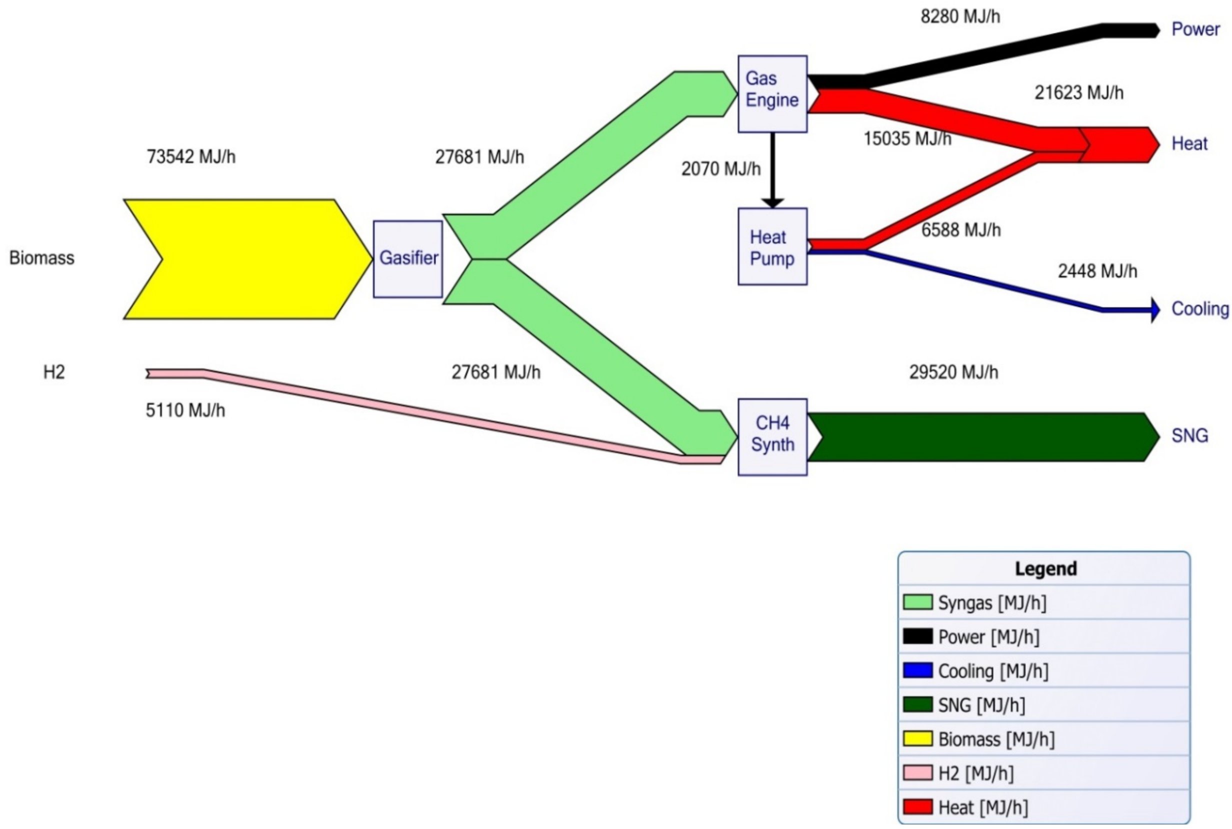

Figure 2.12: Energy balances of the QUAD-50 for one hour of operation.

The data from QUAD-50 case is shown in this table. For an input of 4167.67 kg/hr of straw input, 657.35 kg/hr of SNG can be produced. Table A-4 summarizes temperature, pressure, mass and mole flows of different streams which refer to the numbers used the process diagram (figure 2.4). Stream 1, biomass composition is analyzed in Table 2.1. Stream 3, syngas has more mole components like H_2S, NH3, S and the values are 14.15, 31.73, 0.29 kmol/hr respectively. Stream7 and 8 represents the electricity to the grid and heat pump respectively.

3

Theoretical exergy calculations

Exergy analysis is a method to determine the irreversibilities in the process, providing a more detailed tracking mechanism for energy usage. It is based on the first and second laws of Thermodynamics (Asprion, Rumpf, and Gritsch 2011). In the quad-generation system, exergy of each unit meets the following balance relationship (Hinderink et al. 1996).

$$Ex_{In} = Ex_{Out} + Ex_{Loss} \tag{3.1}$$

For a statically multicomponent stream, three major terms can define exergy: a chemical term, a physical term and a mixing term. So, the total exergy of that multicomponent streams is presented by following equation:

$$Ex = Ex_{Chem} + Ex_{Phys} + Ex_{\Delta mix} \tag{3.2}$$

Where Ex represents the total exergy of the stream, Ex_{Chem} is the chemical exergy of the substances, Ex_{Phys} is the physical exergy and $Ex_{\Delta mix}$ is the exergy of mixing. The system boundaries for the calculation are borders of the facility. Ex_{Input} is defined as the sum of all input streams

$$Ex_{Input} = Ex_{Straw} + Ex_{H_2} + Ex_{Power} \tag{3.3}$$

$EX_{Output}$is defined as the sum of all streams leaving the system boundaries

$$Ex_{Output} = Ex_{Power} + Ex_{Heat} + Ex_{Cooling} + Ex_{SNG} \tag{3.4}$$

3.1 Chemical exergy

The method proposed by Szargut et al. is used for chemical exergy analysis (Szargut, Morris, and Steward 1988). There are some assumptions in calculating the chemical exergy of biomass. Chemical exergy of starch-based and lignocellulosic biomass is calculated from the correlations for technical fuels using the LHV as followed:

$$Ex_{chem} = \beta LHV \tag{3.5}$$

The factor β is the ratio of the chemical exergy to the LHV of the organic fraction of biomass. This factor is calculated from statistical correlations developed by Szargut and Styrylska (Bösch, Modarresi, and Friedl 2012a). The following correlations are used:

$$\beta = 1.0438 + 0.1882 W_H / W_C + 0.01610 W_O / W_C + 0.0404 W_N / W_C \tag{3.6}$$

for $W_O/W_C \leq 0.5$

$$\beta = [1.0438 + 0.1882 W_H / W_C + 0.01610 W_O / W_C + 0.0404 W_N / W_C] / (1 - 0.3035 W_O / W_C) \tag{3.7}$$

for $0.5 < W_O/W_C \leq 2$

The chemical exergy of water is 51 kJ/kg according to its gibbs energy of formation - 237.18 kJ/mol (Bösch, Modarresi, and Friedl 2012b).

3.2 Physical exergy

The physical exergy of a stream represents the total amount of shaft work (or electrical energy) available in that stream. Shaft work is brought by reversible processes from actual conditions (T, P) to thermo mechanical equilibrium at ambient temperature (T_0, P_0) and with heat only being exchanged with the environment at T_0(van Gool 1998; Qian et al. 2009b). A flash calculation at both the reference and the actual conditions is needed in terms of physical energy. Only the contribution of the pure components to the enthalpy and entropy of the mixture at reference and actual conditions is considered to avoid a mixing term. The physical exergy component is given as follows,

$$Ex_{Phy} = \left[L\left(\sum_{i=1}^{n} x_i H_i^l - T_0 \sum_{i=1}^{n} x_i S_i^l \right) + V\left(\sum_{i=1}^{n} y_i H_i^v - T_0 \sum_{i=1}^{n} y_i S_i^v \right) \right]_{T_0, P_0}^{T, P} \tag{3.8}$$

3.3 Exergy change of mixing

For the determination of the exergy change of mixing, the concept of ‘‘property change of mixing” is used. Thus, enthalpy and entropy changes can be calculated to obtain the exergy change of mixing. Enthalpy and entropy changes are calculated by component mole fraction change according to thermodynamics laws.

$$Ex_{\Delta mix} = H_{\Delta mix} - T_0 S_{\Delta mix} \tag{3.9}$$

3.4 Exergy efficiency

In this study, exergitic efficiencies are applied as follows,

$$\eta_{Ex} = \frac{Ex_{Output}}{Ex_{Input}} \tag{3.10}$$

$$\eta_{Ex} = (Ex_{Power} + Ex_{Heat} + Ex_{Cooling} + Ex_{SNG}) / Ex_{Input}$$

$$\eta_{Ex} = \eta_{Power} + \eta_{Heat} + \eta_{Cooling} + \eta_{SNG}$$

Where, $\eta_{Ex,Power} = \dfrac{Ex_{Power}}{Ex_{Input}}$ (3.11)

$$\eta_{Ex,Heat} = \frac{Ex_{Heat}}{Ex_{Input}} \tag{3.12}$$

$$\eta_{Ex,Cooling} = \frac{Ex_{Cooling}}{Ex_{Input}} \tag{3.13}$$

$$\eta_{Ex,SNG} = \frac{Ex_{SNG}}{Ex_{Input}} \tag{3.14}$$

$$\eta_{\text{Irreversibility}} = \frac{\text{Irreversibility}}{Ex_{Input}} \tag{3.15}$$

3.5 Results

The specific exergy of dry biomass varies between 18.8 MJ/kg to 20.23 MJ/kg according to the value of β. The negligible impact of physical exergy streams at the occurring temperature levels of biomass streams in comparison to their chemical exergy is another insight worth noting. Considering this, data from Aspen Plus (modeling tool section) simulation and Eq. (3.1)–(3.9), the exergy of each stream in the whole system is calculated. Table 3.1 represents the exergy of the main material steams for quad-generation energy system. The value of chemical exergy is dominating total exergy content of the stream.

Table 3.1: Exergy of primary streams in quad-generation system.

	Ex_{phy}	Ex_{chem}			Ex_{mix}	Ex
		β	LHV	Ex_{chem}		
Biomass	18.76	1.15	17.65	20.2975	-2.3	36.726
	18.76	1.12	17.65	19.768	-1.96	36.215
Syngas	23	1.1	108.199	119.0189	-4.3	138
SNG	32.32	1.07	418.68	447.9876	-5.6	474.7

For defining individual energy analysis of products, the same five case studies (Rudra, S, Rosendahl LA, and Blarke, MB 2012) introduced in a previous section is considered for calculation. Table 3.2 presents specific exergy inputs of straw, hydrogen and electric power. These numbers are selected according to literature review and Aspen Plus simulation result. Hydrogen is supplied through external source. The remaining process demand electric power is generated through process. Different exergy outputs are also given in Table 3.2.

Table 3.2: Specific energy inputs and outputs

Exergy input (MW)	SNG-0	QUAD-70	QUAD-50	QUAD-30	SNG-100
Biomass	65.655	65.655	65.655	65.655	65.655
H_2	0	1.23	1.41	1.76	2.22
Power	2.4	2	1.5	1.2	1
Sum	68.055	68.885	68.565	68.615	68.875
Exergy Output (MW)					
Power	7.82	5.78	3.91	2.38	0
Heat	18.87	14.62	10.2	8.5	0
Cooling	3.06	1.8	1.156	0.578	0
Bio-SNG	0	8.33	13.94	19.72	30.24
Sum	29.75	30.53	29.206	31.178	30.24

The process efficiency factors are introduced to evaluate the performance, which summarized in table 3.3. η_{Ex} characterize the overall exergy yield of the process regardless of the outputs values. The absolute amount of irreversibility produced are the highest with the scenarios including gas engines for power production (Bösch, Modarresi, and Friedl 2012a). This is consistent with the input requirements. The SNG-100 case stands out in this concern since the produced SNG is not used for further processing and therefore does not contribute significantly to the irreversibility.

Table 3.3: Exergy efficiency analysis for exergy flow

	SNG-0	QUAD-75	QUAD-50	QUAD-25	SNG-100
η_{Ex}	0.662	0.667	0.643	0.685	0.661
$\eta_{\text{Irreversibility}}$	0.337	0.334	0.356	0.314	0.338
$\eta_{Ex,Power}$	0.174	0.126	0.086	0.052	0
$\eta_{Ex,Heat}$	0.420	0.319	0.224	0.186	0
$\eta_{Ex,Cooling}$	0.068	0.039	0.025	0.012	0
$\eta_{Ex,SNG}$	0	0.182	0.306	0.433	0.661

According to the exergetic efficiency calculation, it shows that QUAD-25 has more efficiency then rest of the cases (figure 3.1). SNG-100 has the lowest η_{Ex} with 66.1% In the quad-generation process, when changing the value of the syngas distribution, the production of bio-SNG also changes according to cases. So the exergy efficiency can be changed.

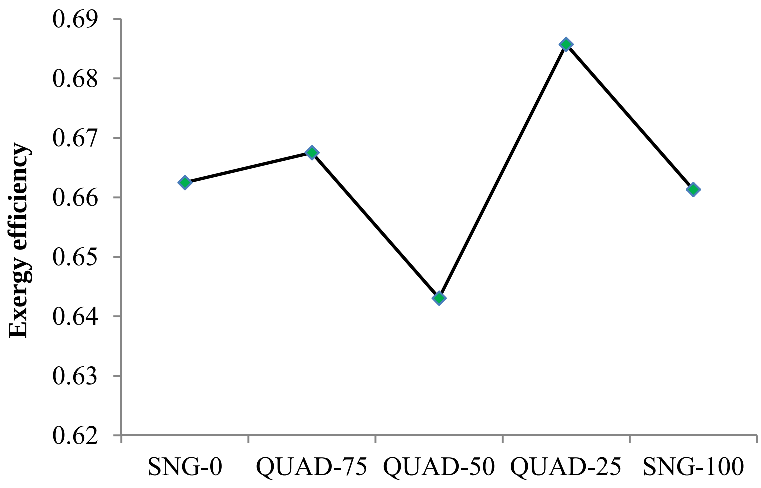

Figure 3.1: Exergy efficiency distribution for different cases

The selection of different cases is the percentage of distributed syngas to CHP and SNG synthesis. In this case, the efficiency is related to the amount of syngas utilized for each production. It is possible to have different exergy efficiencies by selecting some other scenarios, indicating that the current results only yield optimum within the specified scenarios. In order to investigate the input of other scenarios on the exergy analysis, the analysis would have to be repeated for those, following same methodology.

4

LCA analysis of Quad-generation plant

Part of the work has been to carry out a life cycle assessment (LCA) for quad-generation plant. In this chapter, the results and methodology are presented. These have also been included and published in paper 5 (Rudra, S, Kumar, A, and Rosendahl LA 2012).

The conversion of biomass to four different outputs via gasification is a renewable technology with the potential to reduce use of fossil fuels and hence greenhouse gas (GHG) emissions. This study investigates the energy aspects for a new concept of biomass based quad-generation plant producing power, heat, methanol and methane. The quad-generation concept in this study differes from those discussed in previous chapters in that the cooling output stream has been replaced by a liquid biofuel output stream. The plant size for Quad generation pathways is presented in paper 5 (table 1). In this analysis, one product is considered at a time for operation. Circulating fluidized bed (CFB) gasifier and the gas technology institute (GTI) gasifier technologies are used for this quad-generation process. Two different biomass feedstocks are considered in this study. The aim of thisLCA study was to evaluate the energy performance, reduction in GHG and acid rain precursor emission, and use of biomass for different outputs based on demand.

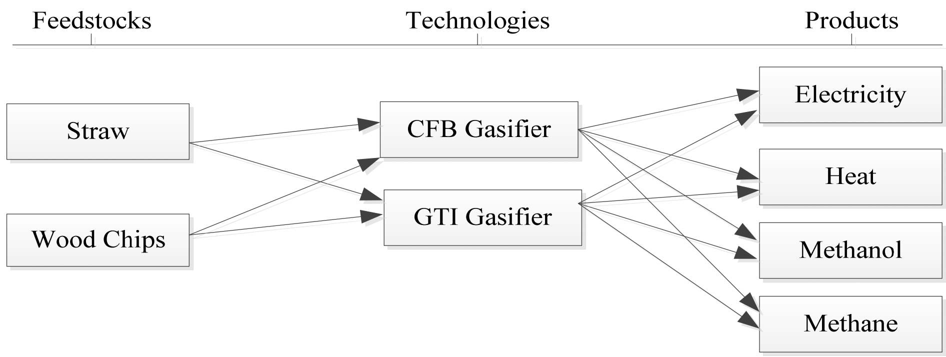

Figure 4.1: Biomass conversion pathways for quad-generation

4.1 LCA methodology:

The size of the plant has considered 1000 dry tonnes per day (dtpd) for both feedstocks. Power, heating, liquid and gaseous fuels are measured in different units (e.g. MJ, kW and m^3); the functional unit is defined as the use of 1 MJ of syngas in either one of these applications. It means the quantity of a service (power, heat, methanol and methane) that is delivered by '1 MJ of syngas' is calculated therefore as the difference between the impacts generated by syngas and reference systems. The explanation of this LCA methodology is published in paper 5 (Rudra, S, Kumar, A, and Rosendahl LA 2012). Figure 4.1 shows the biomass conversion pathways for quad-generation. This study evaluates the NER(Net Energy Ratio) for all quad-generation pathways, a crucial ratio for the assessment of renewable systems. The NERs for the pathways are calculated using Eq. (4.1) (Kabir and Kumar 2011).

$$NER = \frac{\sum E_{out}}{\sum E_{in}} \tag{4.1}$$

where, $\sum E_{in}$ = life cycle non-renewable primary energy input corresponding to the functional unit (FU) of a pathway, and $\sum E_{out}$ = energy available from the FU equivalent amount (MJ) syngas produced from the pathway. It should be noted that this study is based on the lower heating value (LHV) for fuels. Two environmental stressors i.e. net GHG emissions and acid rain precursors (ARP) are considered for emission analysis. These two environmental stressors for a particular conversion pathway arecalculated using Eq. (4.2):

$$\text{Net emission} = \Sigma \varepsilon_{out} \tag{4.2}$$

where, $\Sigma \varepsilon_{out}$ = Life cycle emissions corresponding to the FU of a pathway within the defined system boundary. GHG stressors are reflected to be mainly carbon dioxide (CO_2), carbon monoxide (CO), methane (CH_4), and nitrous oxide (N_2O). GHGs contribute to global warming. The global warming potential (CO_2eq) for these gases are assumed to be 1, 3, 21, and 310 respectively.

4.2 Assumptions of unit processes

The unit processes that have been considered for CFB and GTI technologies are: Biomass production/ Supply (mainly includes seeding, production and distribution of fertilizer, herbicide and pesticide production and distribution, harvesting, manufacturing and decommissioning of all the equipments used in every stage, raking, baling, bale moving and wrapping), biomass transportation (mainly includes loading and unloading, transportation by truck), plant construction, maintenance and decommissioning, plant operation, (mainly includes shredding, plant utilities, ash disposal and regular operation) and quad-productions (mainly includes power, heat, methanol and methane production, methane transportation). The details of the assumptions of unit process are described in paper no. 5 (Rudra, S, Kumar, A, and Rosendahl LA 2012)

4.3 Results

Figure 4.2 presents the energy break down in all unit processes during the life cycle of quad-production for woodchips. The total energy impact for straw and woodchips are comparatively higher than GTI pathways as plant operation and maintenance contributes significantly to the overall energy

Table 4.1: Biomass properties and general assumptions

Properties	straw	Wood chips	Comments/References
Moisture content (%,)	7.5-12	45	These are the moisture contents of as received feedstocks. It is assumed that moisture contents wouldn't change transportation of feedstocks after preliminary processing (Kristensen and Kristensen 2004; Yin, Rosendahl, and Kær 2008)
Bulk density (kg/m3)	130	300	
Lower heating value (MJ/dry kg)	15	10.5	(Kristensen and Kristensen 2004)
Ash content (%)	4		(McKendry 2002)
Plant operating factor			These are conventional operating factors being used for biomass based plants(Callesen, Grohnheit, and Østergård 2010)
Year 1	0.7	0.7	(Kabir and Kumar 2011)
Year 2	0.8	0.8	
Year 3	0.85	0.85	

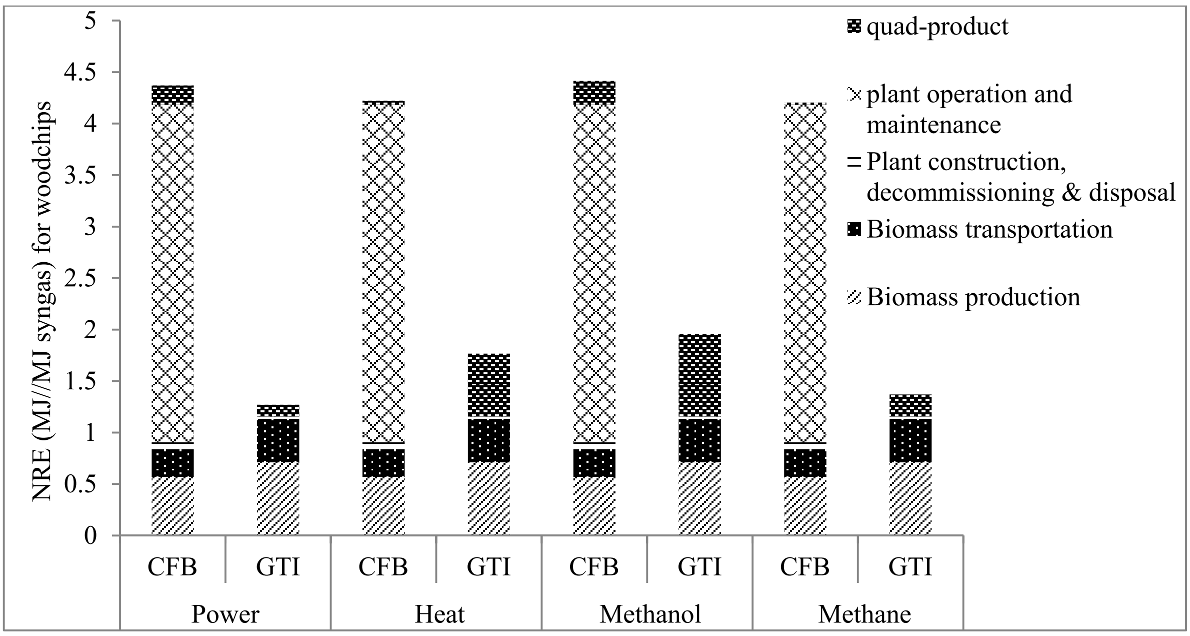

Figure 4.2: NER graphs for both wood chips.

impact. Life cycle energy consumption corresponding to one functional unit is higher for CFB pathways. The main reason is the feedstock pre-treatment and energy input for CFB. So, energy from framing and harvesting is almost double. In addition to that, more transportation distance is needed to be covered. To sum up, NER for quad-production pathways is in the range of 1.3-7.2. In contrast, coal and natural gas based bio-oil production plant demonstrates NER in the range of 0.57-0.67 (Pamela L. Spath and Margaret K. Mann 2000; Pamela L. Spath and Margaret K. Mann 2001).

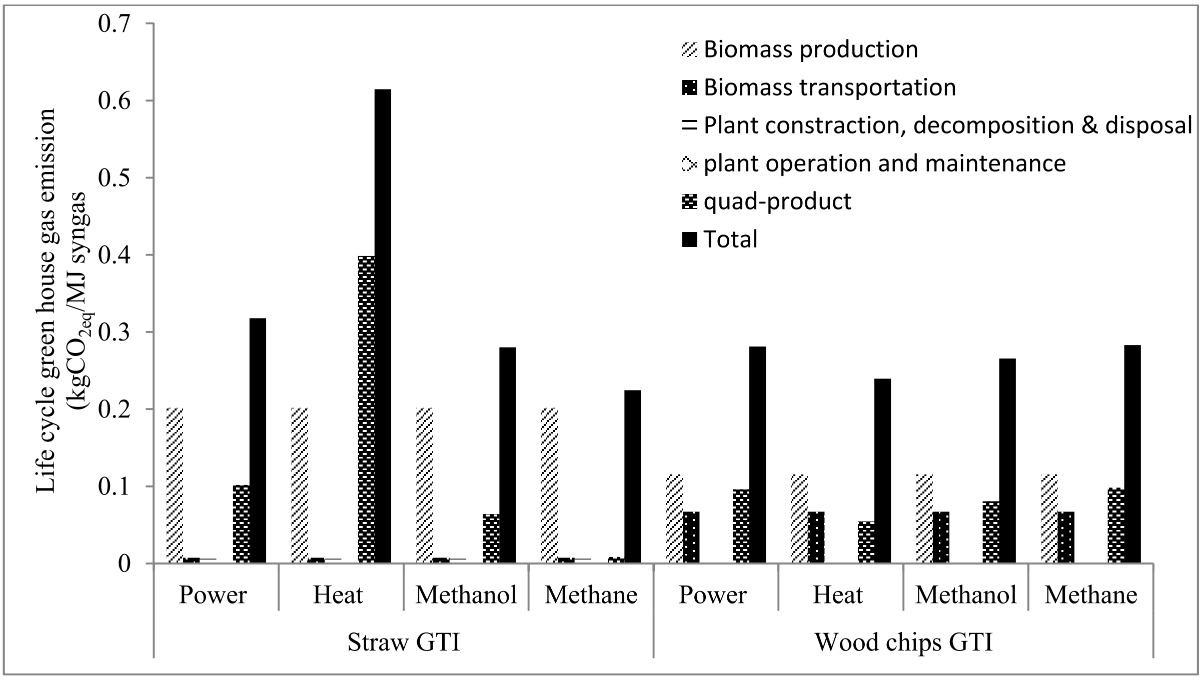

Figure 4.3: Life cycle CO_2 emission from GTI pathways

Life cycle GHG emissions from different pathways are depicted in Figure 4.3 No greenhouse gas (GHG) emissions are generated during biomass growth. Wood transport by truck over short distances is rather efficient and thus the use of diesel and generated air emissions only cause small impacts. Life cycle emission corresponding to one functional unit is higher for CFB straw pathways. The main reasons behind it are that net straw requirement for the same amount of power production is almost double as syngas yield has been assumed to be 50 wt % from triticale straw. The same effect determines the CFB wood chips pathways. A sensitivity analysis is also investigated for this study which is published in paper 5 (Rudra, S, Kumar, A, and Rosendahl LA 2012). Based on this LCA study, GHG and ARP emission intensities for quad-generation production are in the range 0.24 to 4.41 Kg CO_2 eq/NM^3 syngas and 0.03 to 0.84 Kg SO_2 eq/NM^3 respectively.

5

Techno-economic analysis

The objective is to maximize the economic performance of the whole plant while satisfying all design and operational constraints. An understanding of quad-generation process is related to economic evaluation of the process design (Smith, R 2005)

The techno-economic part has three basic roles in the process design.

1. Evaluation of design options: Costs are required to evaluate process design option.
2. Process optimization: the settings of some process variable can have a major influence on the decision –making in the developing flowsheet and overall profitability of the process. Optimization of such variables is usually required.
3. Overall profit availability: The economics of the overall system (quad-generation) should be evaluated at different stages during the design to assess whether the system is economically viable.

In this chapter, two techno-economic analyses are described: techno-economic optimization of a Danish district heating plant according to fuel flexibility and performance, and techno-economic analysis of quad-generation energy system. These analyses also form the basis of paper 3 and paper 4 (Rudra S, Rosendahl LA, and From N 2011; Blarke, MB, Rudra, S, and Rosendahl, LA 2013)

5.1 Techno-economic optimization of a Danish district heating plant

Brovst is a small district in Denmark. The present use of fossil fuels in the Brovst DHP (district heating plant) represents an increasing environmental and climate-related load. Therefore, an investigation is made to reduce the use of fossil fuels for district heating system and make use of the local renewable resources (Biogas, solar and heat pump) for district heating purposes. Figure 5.1 shows the heat demand of Brovst district heating plant. In this thesis, the techno-economic assessment is achieved through the development of a suite of models that are combined to give cost and performance data for this district heating system. Local fuels are analyzed for different perspectives to find the way to optimize the whole integrated system in accordance with fuel availability and cost. energyPRO ("energyPRO Users Guide, EMD International A/S, Aalborg, < Www.emd.dk >" 2010), is used to analyze the integration of a large scale energy system into the domestic district heating system. A model of the current work on the basis of information from the Brovst plant (using fossil fuel) is established and named as a reference option. Then four other options are calculated using the same procedure according to the use of various local renewable fuels known as "Biogas option," "Solar option," "Heat pump option" and "Imported heat option"(Rudra S, Rosendahl LA, and From N 2011) page 3-4.

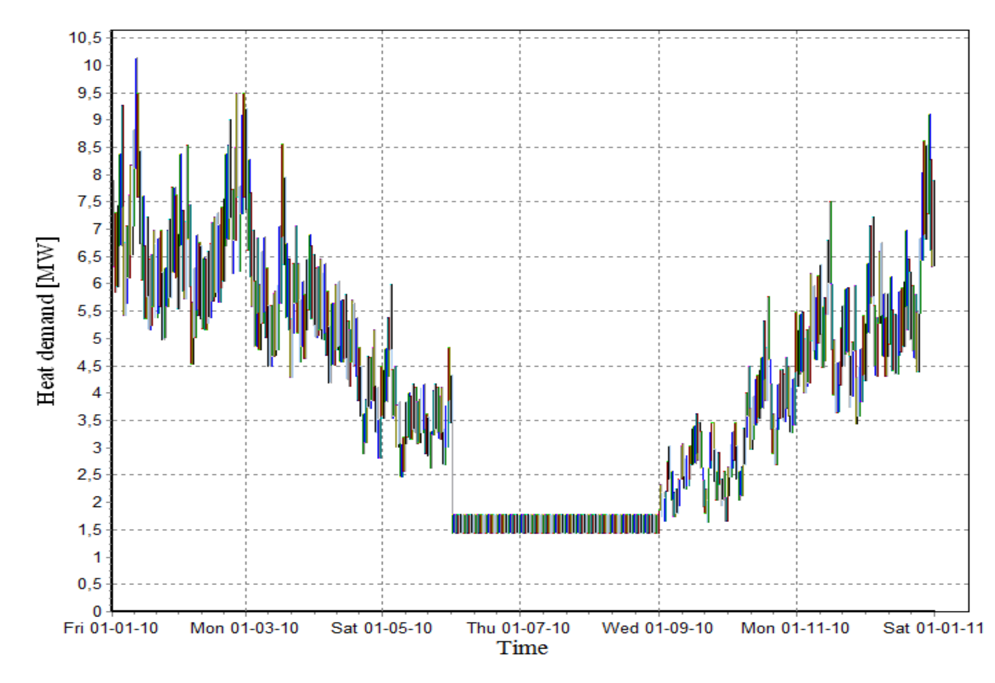

Figure 5.1: Heat demand of Brovst DHP during whole year.

5.1.1 Method

The energyPRO computational procedure is used for this techno-economic optimization ("energyPRO Users Guide, EMD International A/S, Aalborg, < Www.emd.dk >" 2010) and this software tool is used for modeling energy systems including district heating plants (Hendriks and Blok 1996). To secure productions in the most favorable periods, energyPRO works in a way, which is not performing chronologically but producing in the most favorable periods. In the case of energyPRO, before accepting a new production it checks the new production does not create overflow in the thermal stores in the future – taking into account the already planned productions. In the simulation of thermal storage calculation, it needs the following to be defined: volume, temperature in the top and bottom, capacity, operation restricted to period, annual non-availability periods and storage loss. So for each future time interval the following formula is used:

$$ST_e[i,t] = ST_b[i,t] + (O_{ap}[i,t] - DE[i,t]) \times dt \tag{5.1}$$

Where, ST_e and ST_b are the end and beginning content in the storage for a time interval.

O_{ap} is output already planned.

DE is demand.

dt is length of time interval

Acomplete description of this procedure of calculation has been described in paper no. 3 (Rudra S, Rosendahl LA, and From N 2011) page 2-3. Figure 5.2 shows the different steps of this techno-economic optimization.

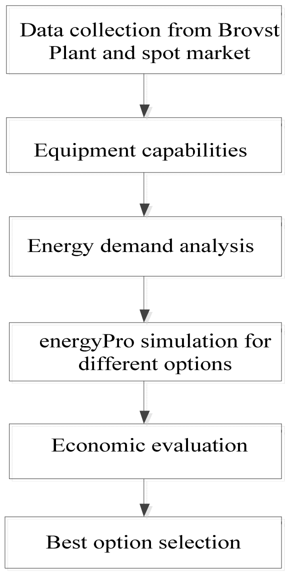

Figure 5.2: Steps of techno-economic optimization.

5.2 Techno-economic analysis of quad-generation energy system

An advanced quad-generation concept is presented, an operational dispatch model is developed and optimized using mixed-integer linear programming techniques, and analyzed on an hourly basis with respect to techno-economic consequences, including energy balances, costs, and environmental impacts. It is found that quad-generation provides a valid technological concept for complete 100 % renewable local energy systems that perfectly integrates multiple processes to supply local energy requirements, even the need for transportation fuels (Blarke, MB, Rudra, S, and Rosendahl, LA 2013).

5.2.1 Methodology and assumptions

The quad-generation concept (Rudra, S, Rosendahl LA, and Blarke, MB 2012) is modeled using COMPOSE (Blarke, MB 2013; Connolly et al. 2010) , which allows for techno-economic operational optimization using mixed-integer linear programming (MILP) of complex cogeneration plants. The MILP program is formulated according to the standard formulation presented in the following equation:

$$\min\ f(x) = \sum_{\text{hour}=1}^{8760} \text{operational costs}_{\text{year, hour}} \qquad (5.2)$$

$$s.t.\ \text{linear constraints and bounds, and certain integrality constraints}$$

Consequently, COMPOSE identifies the plant's optimal operational strategy by minimizing the economic cost of heat and cooling production for each year of operation under constraint of annual and hourly deterministic projections for energy requirements, O&M costs, unit capacities, and electricity and SNG markets. All financial costs are excluded and if there are CO_2 credits, if any, are not adopted. There is no capacity constraint on SNG sold and electricity sold/bought. A detailed description of the modelling framework and the operational optimization programming is provided in (Blarke and Dotzauer 2011b). The plant is optimized for operation over a 20 year planning period from 2013-2032 under which it is stipulated that all investments are fully depreciated. The district heating requirements are based on historical requirements from an existing and typical distributed CHP plant with 1260 consumers (Blarke, MB and Rudra, S 2012), while the district cooling requirements are loosely estimated based on what could be the space cooling requirements of the area's commercial buildings. Projected annual fuel and electricity costs are based on official projections published by the Danish Energy Authority ("Danish Energy Authority (In Danish: Energistyrelsen), Assumptions for Economic Analyses in the Energy Sector (Danish: Forudsætninger for Samfundsøkonomiske Analyser På Energiområdet)" 2011). Investment costs and O&M costs are based on today's technology according to (J. Møller Jensen and J.J. Møller 1995). All the key parameters are presented on paper no 4 (specially from table1 – table 4 and in figure 1) (Blarke, MB, Rudra, S, and Rosendahl, LA 2013) that constitute the techno-economic constraints.

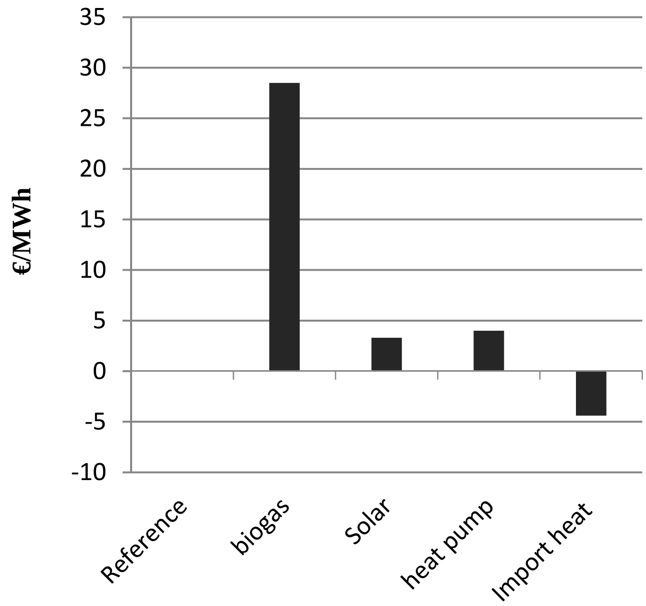

Figure 5.3: Variation of heat production price according to different fuel options

5.3 Results

5.3.1 Techno-economic analysis of Danish district heating plant

Locally available renewable energy resources should be considered when an energy system is designed and analyzed by a systems analysis model, yielding results on an aggregate annual level as well as on an hourly basis. By getting individual solutions from simulations, this study combines all the economic outcomes for making a decision regarding fuel selection and engine performance. Figure 5.3 shows the different heat production price according to the fuel options. The best option for saving money is the Biogas option where it is possible to save 28.53 €/MWh considering the reference case as zero savings.

This work concludes that the best solution is to combine a gradual expansion of the district heating production with the biogas option where 66% heat is produced by using biogas, 13% natural gas engines and 21% natural gas boilers. The next best option is the Heat pump option as it uses less fossil fuel than the solar option. Furthermore, this municipality considers a joint distribution and production of geothermal heat to be established as a municipal cooperation which may serve the nearby localities. It also helps to reduce the heat production from natural gas in Biogas option.

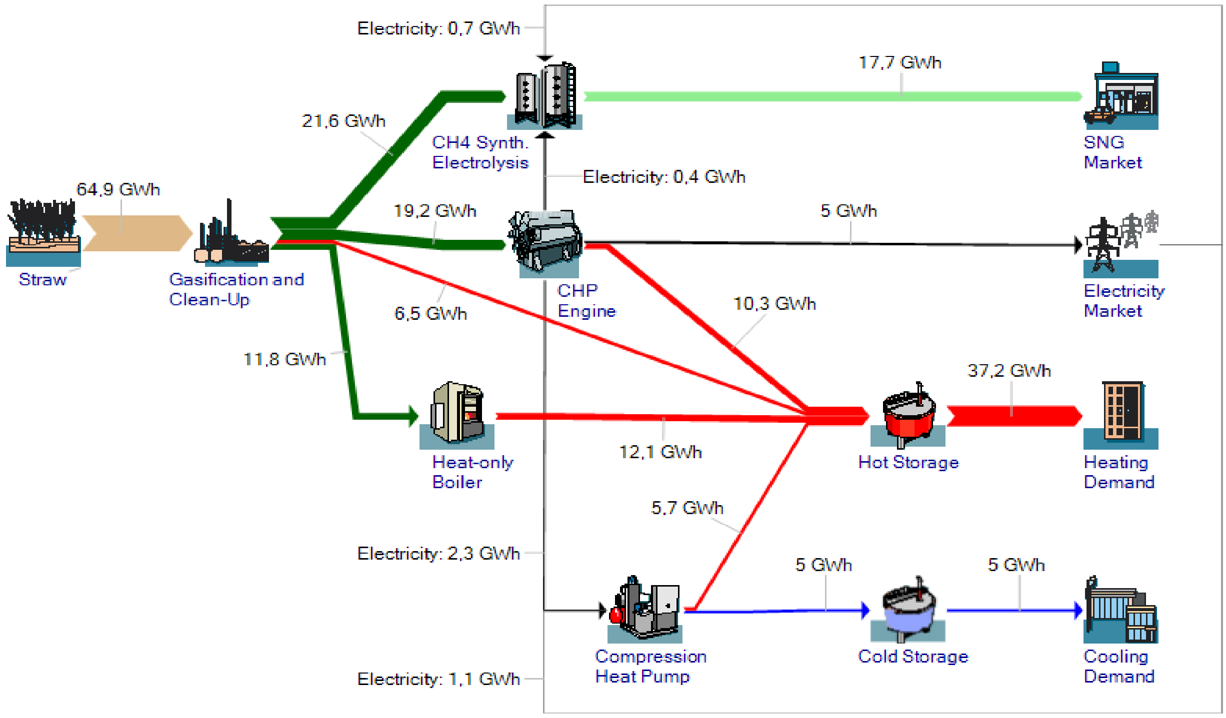

Figure 5.4: 2013 energy balance of Quad-concept for optimal operation.

5.3.2 Techno-economic analysis of quad-generation plant

Figure 5.4 illustrates the Quad-concept's energy balance in 2013 optimized for least-cost operation. The overall direct fuel-to-energy efficiency is 97%. Straw consumption totals 64.9 GWh, or 16,000 tons of straw, corresponding to the annual output from 5,000 ha of agricultural land, corresponding to 0.2% of

Denmark's farmed land in 2010. The plant sells 5 GWh electricity, purchases 1.8 GWh electricity, and sells 17.7 GWh SNG. The heat pump's share of total heat production is 16%, the CHP engine's share is 30%, while the heat-only boiler's share is 35%.

The base sets of assumptions result in a negative economic internal rate of return (EIRR) of -1.6% and it is described in graphical presentation in paper 4. The system-wide CO_2 emissions reduction declines from 9,638 ton per year in 2013 to 3,672 ton per year in 2032. In fact, the quad-concept results in negative system-wide CO_2 emissions as a result of the replaced natural gas from sold SNG and the replaced fossil fuel in central electricity generation from sold electricity.

CHP and Quad operation by their "intermittency-friendliness" coefficient 'for each year of operation is also introduced in paper 4*Rc'* (Blarke, MB, Rudra, S, and Rosendahl, LA 2013) . The net electricity requirement is defined as the electricity demand minus the intermittent electricity production. *Rc* serves to evaluate the marginal "goodness" of a plant's or end-user's response to variations in net electricity requirements ranging from -1.0 to 1.0. It is found that *Rc* is *lower* for the quad-concept, making it *less* intermittency-friendly, which is due to the Quad-concept's additional operational constraints.

6

Conclusion

The objective of this study is to design and system analysis of quad-generation plant based on gasification of biomass, with focus on the following issues:

1) Integrating the district heating plant with quad-generation energy system
2) Optimizing a district heating plant according to energy efficiency and fuel flexibilities.
3) Improving quad products yield per unit of biomass input.
4) Techno-economic analysis of a 100% renewable energy plant for flexible local production of electricity, heating, cooling, and bio-fuels.

Considering the main areas identified in figure. 1 for the structure of the thesis, the following conclusions can be summarized:

System design:

A quad-generation system is designed according to the fuel demands of the specific plants. The attempt of this system model is to provide an overview of possible technical outcomes of a new green system regarding fuel production efficiency and exergy performance. It also endeavors to select the best case among the possible alternatives, in accordance with explicit technical objectives, i.e., efficiency and exergy analysis. In case of utilizing different simulation results, SNG-0 case is more appropriate for the winter as the demand for heating rises in this season, while the QUAD-25 case would be more appropriate in the summer because it can produce more bio-SNG and still produce some power, heat and cooling. During excess power production from wind and a lower price for heat from other heating plants, SNG-100 would be a good option for a quad-generation plant. The quad-generation system allows full flexibility to operate in these optimal modes.

In this context, this work investigated a process that converts biomass into bio-SNG, which is equal in quality to fossil-derived natural gas and it is possible to utilize the existing national natural gas grid. With the increasing market share of gas engines in the transport sector, fossil fuels could therefore be partially substituted by a renewable fuel that is neutral in greenhouse gas emissions.

System optimization

Optimization of DHP:

The purpose of the techno-economic analysis presented in thesis is to optimize the Brovst DHP according to reduction of heat production price. The different combinations are ordered to provide for a qualified basis to make a preliminary sorting of the suggestions. By getting individual solutions from simulations, this optimization work concludes that the best solution is to combine a gradual expansion of the district heating production with the biogas option. The second option is the Heat pump. This conclusion is valid both in the present systems, which are mainly based on fossil fuels, as well as in a potential future system based on 100 % renewable energy.

Techno-economic optimization of quad-generation:

Thermodynamic analysis investigates the techno-economic performance of an innovative straw-fuelled quad-concept that produces all four basic energy services: electricity, heat, cooling, and liquid or gaseous fuels. This can be an attractive sustainable energy option for island-mode operation and for high-efficiency distributed generation systems. In terms of intermittency-friendliness coefficient *Rc*, both quad-generation and reference CHP operation are hit by falling rates of "goodness". In the years ahead, such further advanced quad-generation may provide a pathway for optimal co-existence between the biomass energy resource and intermittent renewables, such as wind power.

System analysis:

The LCA analysis investigated the energy aspects for the biomass based quad-generation plant producing power, heat, methanol and methane. The net energy ratio (NRE) for six different pathways having the range of between 1.3 – 7.2**.** The lowest limit corresponds to the wood chips-based power, heat, methanol and methane production pathway using GTI technology. Scenario 1 for sensitivity analysis (Rudra, S, Kumar, A, and Rosendahl LA 2012) consider excluding the farming and harvesting inputs. Hence, the feedstocks can be regarded as waste material energy need not to be allocated to feedstocks as it was in the base case By increasing the share of wind power in total energy system, reducing the use of fossil fuels use in energy production and replacement of those fossil fuels with domestic biomasses will represent the main means of GHG emissions saving in the future energy system.

6.1 Future work

The result that is published in this thesis is an attempt to consider fundamental issues of biomass gasification process design, operation and optimization of the proposed quad-generation system. This work also raised several issues that pave the way towards further development of quad generation and beyond.

This thesis work has been achieved using simulation models and some system analyses. But it has not validated with experimental test. The analysis has demonstrated that quad-generation, particularly the process simulation, can play an important role in meeting flexible fuel demand. However, in order to arrive at detailed conclusions, it is necessary to consider a much wider range of technical options and practical impediments. In this regard, the following studies are recommended.

- **Integration of gasification unit methanol synthesis process.**

The new and novel way of Methanol production by utilizing the captured CO_2 from plant and H_2 from electrolysis of electricity from wind energy, could introduced as a new and novel energy conversion process. This type of energy system (figure 6.1) integrating methanol synthesis into a typical local district heat plant would be a coherent solution for the challenges in the future energy supply. Methanol synthesis will in this context serve to close a carbon loop, where it is possible to stop emissions of CO_2 and help to minimize the effects of global warming. In addition, methanol is an attractive storage medium, as it keeps the advantages of a liquid fuel, which can be used both in traditional combustion engines. This concept attempts to solve some of the fundamental problems with the future energy situation.

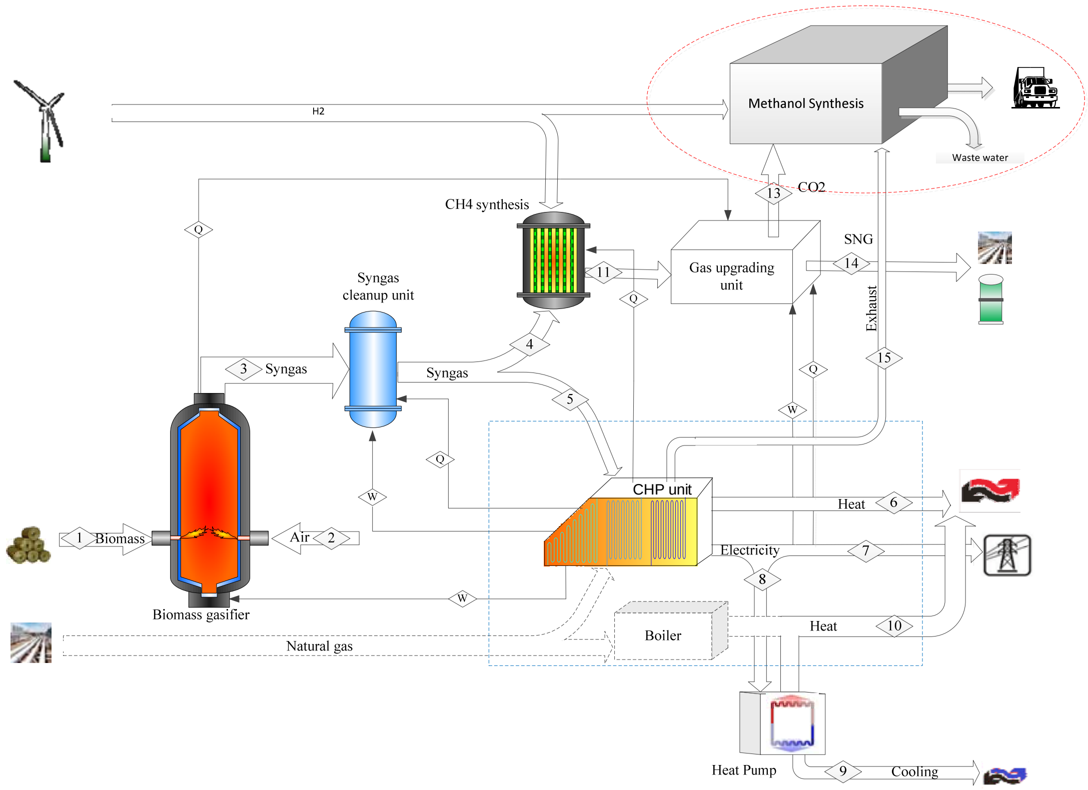

Figure 6.1: Quad-generation energy system including methanol synthesis.

- **Experimental analysis of a lab scale system.**

To validate the steady state thermodynamic equilibrium model, it would be a timely approach to build a small lab to scale biomass-gasification-based quad-generation system, which can be carried out by utilizing simulated result of this present work.

- **Heat integration and pinch analysis**

There are some waste heat sources (gasification reactor, gas engine exhaust) and some stream needs heating (drying biomass) in quad-generation process. To integrate waste heat for heating purpose inside the process, a pinch analysis has to be conducted.

- **Integration of quad-generation with SOFC**

SOFC (Solid oxide fuel cell) can be coupled with quad-generation to improve thermal efficiency and reduce CO2 emission per unit energy production. Both syngas and hydrogen from electrolysis can be used to run SOFC.

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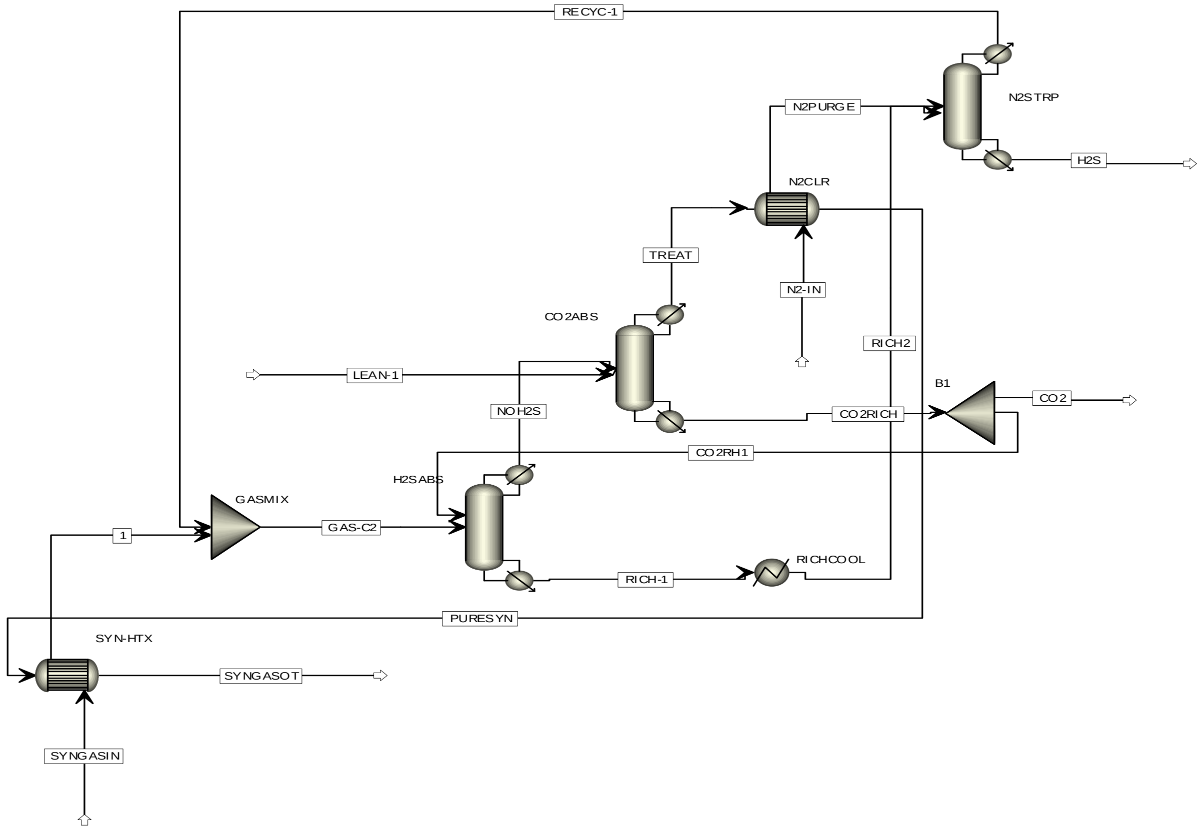
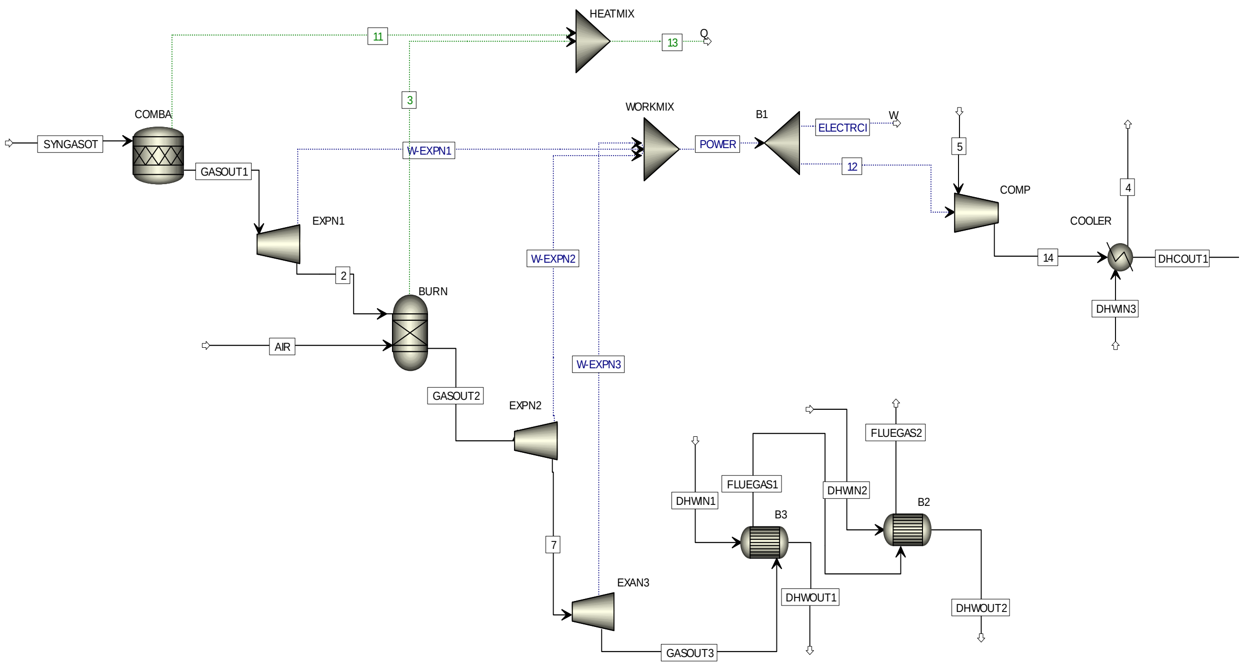
Appendix

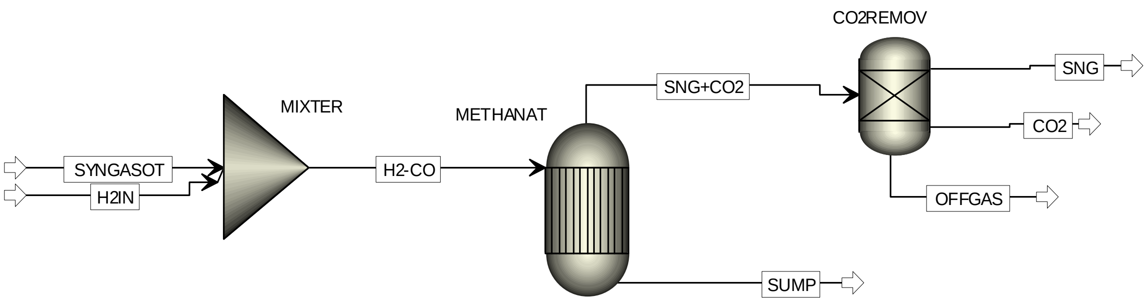


a) gas clean up

Figure A -1: Process flowsheet a) gas clean up, b) Power, heat and cooling production unit, and c) Bio-SNG synthesis unit



b) Power, heat and cooling production unit



c) SNG synthesis unit

Figure A -1: Process flowsheet a) gas clean up, b) Power, heat and cooling production unit, and c) Bio-SNG synthesis unit

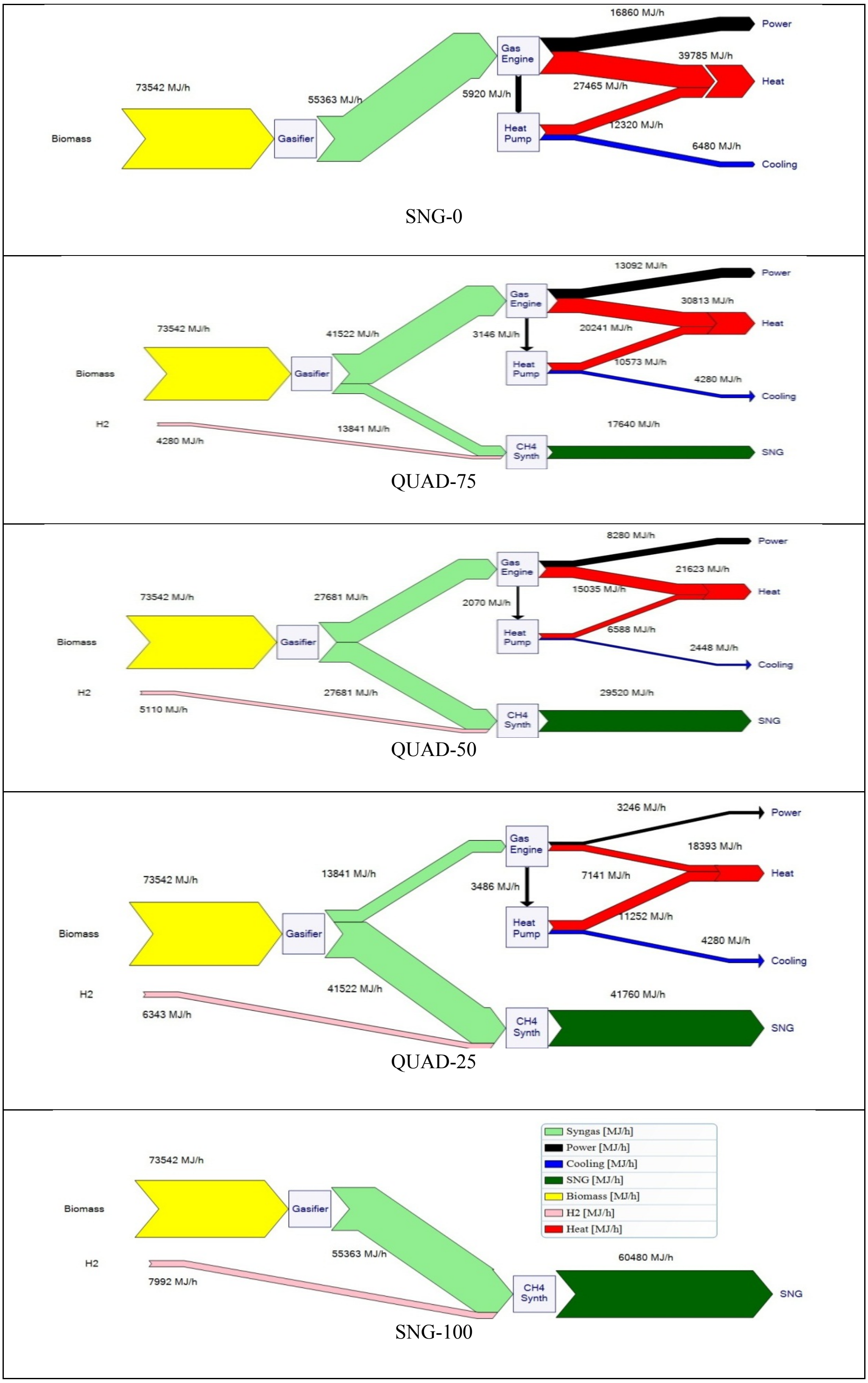


Figure A-2: Sankey diagrams for energy balances of the SNG-0, QUAD-75, QUAD-50, QUAD-25 and SNG-100 cases for one hour of operation.

Table A-1: Description of the reactor blocks utilized in the simulation

Block ID	Aspen floowsheet Name	Description
RYIELD	BIOMASS	Yield reactor-converts non-conventional biomass to conventional components by using FORTAN statement. Yields (per mass of total feed) have to be specified during simulation.
RSTOIC	DCOMBIOM	Reaction kinetics are unknown or unimportant. This type of reactor can model reactions occurring simultaneously or sequentially. Specify operating conditions, reactions, reference conditions for heat of reaction calculations, product and reactant components for selectivity calculations
MIXTER	MIXTER	Mix of air and decomposed biomass feed from DCOMBIOM and feed to GASIFIER.
RGIBBS	GASIFIER	RGibbs can calculate the chemical equilibrium between any number of conventional solid components and the fluid phases. Specify reactor operating conditions and phases to consider in equilibrium calculations
SEPRATOR	SEPARATOR	Separates gases from ash by specifying split faction.
Columns (REDRAC)	CO2ABS, H2SABS	It simulates all types of multistage vapor-liquid fractionation operations. Specify basic column configuration and operating conditions.

Table A-2: Compositions straw gasification unit for the quad-generation plant model using Aspen Plus. Stream name refer to figure 2.9 and figure A-1.

Stream name	AIRFUELM	AIRGAS	DCOMFEED	DRYBIOM	GASFIED	GASIOUT	SYNGSOUT
Mass flow (kg/hr)	8135.6	3968.9	4166.676	4166.676	4166.676	7209.681	7209.681
Mole Flow Kmol/hr)	400.312	136.81	263.504	0	365.032	393.27	393.277
Mass fraction							
H2O	0.147	0	0.328		0.285	0.159	0.159
CO	0.065	0	0.145		0	0.052	0.052
CO2	0	0	0		0	0.022	0.022
O2	0.161	0.27	0.021		0.142	7.38E-16	0
N2	0.401	0.72	0.005		0.142	0.457	0.457
CH4	0.048	0	0.107		0	0.047	0.047
C2H6	0	0	0		0	6.31E-05	6.31E-05
C2H4	0	0	0		0	1.41E-05	1.41E-05
C2H2	0	0	0		0	8.48E-08	8.48E-08
C3	0	0	0		0	1.83E-07	1.83E-07
C4	0	0	0		0	4.76E-10	4.76E-10
H2S	0.066	0	0.148		0	0.068251	0.068
NH3	0.074	0	0.166		0	0.006996	0.006
SULFUR	0.001	0	0.002		0.142	1.05E-09	1.05E-09
CARBON	0	0	0		0.142	8.23E-22	0
STEAM	0	0	0		0	0.159587	0.159
SO2	0	0	0		0	5.29E-08	5.29E-08
NO2	0	0	0		0	7.71E-19	0
SLAG							
H2	0.032	0	0.072695		0.142	0.0257	0.025

Table A-3: Stream compositions gas clean up unit for the quad-generation plant model using aspen plus. Stream name refer to figure 2.9 and figure A-1.

Stream name	SYNGASIN	1	GAS-C2	LEAN-1	N2-IN	NOH2S	PURESYN	SYNGASOT	TREAT
Mass Flow	6869.487	6869.48	6869.48	231.889	12	6869.48	7101.376	7101.376	7101.376
Mole Flow	367.0334	367.033	367.033	6.803	0.428	367.033	373.837	373.837	373.837
Mole Fraction									
N2	0.348952	0.348	0.3489	0	1	0.3489	0.342601	0.342601	0.342601
O2	0	0	0	0	0	0	0	0	0
CO	0.148308	0.148	0.1483	0	0	0.1483	0.145609	0.145609	0.145609
H2	0.380738	0.380	0.3807	0	0	0.3807	0.373808	0.373808	0.373808
CO2	1.84E-03	1.84E-03	1.84E-03	0	0	1.84E-03	1.81E-03	1.81E-03	1.81E-03
NH3	6.23E-03	6.3E-03	6.23E-03	0	0	6.23E-03	6.12E-03	6.12E-03	6.12E-03
H2S	0.110827	0.110	0.110	1	0	0.110	0.127	0.127	0.127
CL2	0	0	0	0	0	0	0	0	0
CH4	6.30E-04	6.30E-04	6.30E-04	0	0	6.30E-04	6.19E-04	6.19E-04	6.19E-04
H20	2.45E-03	2.45E-03	2.45E-03	0	0	2.45E-03	2.40E-03	2.40E-03	2.40E-03
C2H4	2.39E-05	2.39E-05	2.39E-05	0	0	2.39E-05	2.34E-05	2.34E-05	2.34E-05
C2H6	0	0	0	0	0	0	0	0	0.00E+00

Table A-4: Parameters of the main points of the quad-generation system.

Stream	Temp (^oC)	Pressure (bar)	Mass flow (kg/h)	Mole flow (kmol/h)								
				N2	O_2	CO	H_2	CO_2	H_2S	CH_4	H_2O	C_2H_4
1	25	1.01	4167.67	-	-	-	-	-	-	-	-	-
2	25	1.01	1000	32	96.015	-	-	-	-			
3	1205.1	28	7209.68	32.66	98.24	16.84	86.87	16.84	14.14	21.7	59.04	0.4
4	650	25	7625	-	10.2	19.35	56.66	0.84	0.71	18.66	41.02	0.4
5	650	25	3812.5	-	10.2	19.35	56.66	0.84	0.71	18.66	41.02	0.4
6	90	1.01	2000	-	-	-	-	-	-	-	55.51	-
7	-	-	-	-	-	-	-	-	-	-	-	-
8	-	-	-	-	-	-	-	-	-	-	-	-
9	5	1.01	362.35	-	-	-	-	-	-		55.35	-
10	95	1.01	502.72	-	-	-	-	-	-	-	15.63	-
11	614.58	1.01	7689.24	-	-	6.49	0.04	37.86	0.02	48.68	36.47	0.49
12	100	1.01	42	-	-	-	31.87	-	-	-	-	-
13	270	20	257.29	-	-	6.49	0.043	37.86	8.35	-	67.64	0.49
14	270	20	657.35	-						30.24		-

Paper 1

Proposal of a biomass based Quadgeneration system for power, heat, cooling and SNG production.

Rudra, S.; Rosendahl, L; Blarke MB.

International Journal of Green Energy (under review)

Design and process analysis of a biomass-based quad-generationplant for combined power, heat, cooling, and synthetic natural gas production

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***Abstract*—A new concept for upgrading distributed co-generation plants to quad-generation plants, which combines the production of power, heating cooling and synthetic natural gas (SNG), is designed and analyzed. Five cases with SNG production ranging from 0 to 100 % of total energy outputs are designed to simulate different modes of operation. The quad-generation system is simulated using ASPEN PLUS and described by simulating different portions of the system. This paper also describes the new process, which is of particular interest for improving the total first law efficiency. With this system, it is possible to increase the efficiency of natural resource utilization, minimize the environmental impact in distributed generation, and, by providing flexible operation, better support the integration of intermittent renewables such as wind power. Strawis used as a biomass feedstock for this simulation. The net energy efficiency is used to evaluate the performance of the quad-generation system. The results show that the proposed system could be most efficient in the QUAD-25 case, providing 89.8 % net energy efficiency, which is almost 4.1% higher than the SNG-0 case. Based on the flowsheet simulation, this energy assessment compares the proposed quad-generation system to the existing district heating system.**

Keywords*—*Quad-generation; straw; SNG

I. INTRODUCTION

The increasing demand for energy, environmental concerns, and trends toward the deregulation of energy markets have become integral parts of energy policy planning. Flow-based energy resources are largely incompatible with the current energy infrastructure, and a new and more complex structure is required to produce a more sustainable energy system. The development of energy-efficient production technologies has made cogeneration and tri-generation possible (Blarke, 2012; Buoro, 2011) and now, the development trend is moving towards quad-generation and poly-generation. Meeting the future demand for power, heat, cooling, and bio-fuels with highly limited and fluctuating resources will require carefully planned allocation of the available renewable resources and a highly flexible system. All of these aspects have added new dimensions to energy planning. One of the renewable resources that could fulfill all of these demands is biomass, and one of the most efficient ways of utilizing this biomass is gasification (Schmidt, 2010). Thus, this study proposes and studies a novel hybrid configuration for a biomass-based quad-generation system. It shows how the plant owners can utilize their total capacity by producing different fuels according to the local demands.

In Denmark, there are a substantial number of biomass-fired district heating plants, and approximately 10 straw- or wood-chip-fired decentralized combine heat and power (CHP) are also in operation. The rest of the decentralized CHP plants are fuelled by natural gas. More than 15 PJ of biomass and 8 PJ of natural gas were utilized in heating plants, and 30 PJ of natural gas and 18 PJ of biomass were utilized in decentralized CHP plants (Danish Energy Agency, 2012). From this starting point, a scenario framework has been suggested in which the Danish system is converted to 100 percent renewable energy sources (RES) by the year 2060, including reductions in space heating demands by 75 percent (Lund, 2010).The European Commission has also developed political strategies to increase the share of renewable and sustainable energy in fulfilling the overall energy demand (European Commission, 2007; Hetland, 2009).

Biomass conversion can be divided into two main pathways: thermochemical conversion and biochemical conversion (Turkenburg, 2000). The main thermochemical pathway for dry biomasses can be divided into combustion, gasification and pyrolysis (Brown, 2004). Gasification converts the biomass into a syngas that can subsequently be used to generate heat and power or converted into fuels or other chemicals (Faaij, 2006). In this study, the existing methodology is replaced by gasification as it is one of the most efficient conversion methods.

The most stable state-of-the-art gasification technologies combined with the possibilities of cogeneration through the gasification of biomass have been described and compared in a Danish context (Ahrenfeldt, 2012), and it has been shown that the thermal gasification of biomass is both highly flexible and efficient. There are a number of scientific publications that address some novel concepts for polygeneration system design and energy analysis using different input fuels (Qian,2009; Gao, 2008).These papers found that system integration with gasification technology made a significant contribution to the improvement of performance. The concepts of polygeneration and energy integration have been described using various examples of systems (Yu, 2010), and some papers have published the mathematical modeling and simulation of polygeneration energy systems (Li, 2010; Li, 2008; Wang, 2009; Paviet, 2009); however, these papers focus on the evaluation of new plants and technologies concerning the configuration design of the processes. With the aim of achieving higher efficiency and lower emissions, innovations in both power generation technologies and process integration strategies were taken into account in the development of a fully integrated plant (Jhuma.2010; Rudra, 2010; Hoffmann, 2011; Ilic, 2012).The high efficiency of small-scale biomass gasification quad-generation based on gas engines provides an opportunity for converting natural gas fired heating plants into efficient quad-generation plants that have not been used previously. Natural gas-fuelled gas engine quad-generation plants can either be converted into pure biomass-based plants or dual fuel plants, operating on producer gas, natural gas or mixtures of both. The main advantage of the conversion of such plants is that the gas engine is already installed, and this is normally a major part of the total investment. For high chemical conversion and effective energy utilization, a new biomass-based quad-generation system using existing gas engines and an additional synthesis unit for power, heat, cooling and SNG production is proposed in this paper.

Research into large-scale investment planning to convert existing plants to quad-generation energy systems is limited, albeit clearly crucial for strategic policy-making in regions and countries. This paper includes different scenarios according to the fuel demands of the specific plants and attempts to provide an overview of possible technical outcomes of a new green field quad-generation system regarding fuel production efficiency. It also endeavors to select the best case among the possible alternatives, in accordance with explicit technical objectives, i.e., efficiency.

II. Scope of this work

The Brovstdistrict heating plant (DHP) is one of the district heating plants in the Jammerbugt municipality in Northern Denmark. Fig.1 shows the heat demand of the Brovst DHP. Scenario 1 represents the existing capacity of the Brovst DHP. The distance between the heat demand curve and scenario 1 line embodies the free capacity. In the summer, especially from June to August, heat demand is lower than in the rest of the

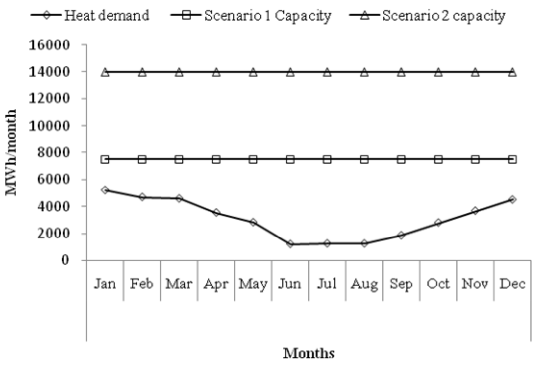


Fig.1 Heat demand and total capacity over a year for the Brovst DHP

year. During this period, it is necessary to shutdown heat production from the engine. The motivation of this work is to utilize this free capacity between the plant capacity and the actual production by upgrading the existing system to quad-generation. It will also possible to scale up the production like scenario 2 in fig. 1.Scenario 2 line represents the extended capacity for the quad-generation.

Both scenarios include power, heat, cooling, and fuel demand and assumed that both are constant. Feedstoke selects 100 ton of biomass per day according to satiate scenario 2 (own calculation). By installing a quad-generation system, the plant can satisfy public demand for heat while also producing power, cooling and SNG according to the demand and the market value of each. The use of fossil fuels is also associated with many concerns, among which are the security of the supply and the resulting air pollution. One of the ways to reduce the transportation sector's dependency on fossil fuels is to use biofuels from quad-generation plants. In this region, a large amount of power is produced by wind farms, but the output is variable according to the availability of wind. In cases of excess power production from wind, the excess can be utilized to produce H_2 for CH_4 synthesis. Therefore, a quad-generation power plant can be used in conjunction with wind energy because it has flexible output.

III. System description and design

A. *Description of existing plant*

The Brovst DHP uses natural gas for the production of heat and power. Heat demand is approximately 37,200 MWh/year. The system inside the dotted line in Fig.2 represents the existing plant. Presently, it has two natural gas generator sets with an output of 3.1 MW of power and 4.1 MW of heat, with the power being sold to the national grid. It also has two condensing hot water boilers with a total of 8.15 MW of heat production. A 1600 m^3 storage tank has also been installed in this plant.

B. *Description of proposed quad-generation plant*

A quad-generation system is proposed, as described by the flowsheet in Fig. 2.

The process is described by the following steps:

1. The biomass is gasified in the presence of air at atmospheric pressure.
2. The syngas leaving the gasifier will be cooled and cleaned by a gas cleanup unit. The particulate matter is removed from the raw syngas exiting the gasifier using a cyclone collector and a candle filter system.
3. One of the streams from the syngas cleanup unit will be sent to the engine for power and heat production, while a compression heat pump is introduced. It is a flexible compressor-driven unit able to produce both cooling and heating.
4. The synthesis gas can contain a considerable amount of methane and other light hydrocarbons, representing a significant part of the heating value of the gas. Therefore, another stream from the gas clean-up section enters the CH_4 synthesis section to be converted to CO and H_2 driven by the addition of steam over a catalyst at

high temperatures. Subsequently, it maintains a proper

- QUAD-50: In this scenario, 50% of the bio-syngas is

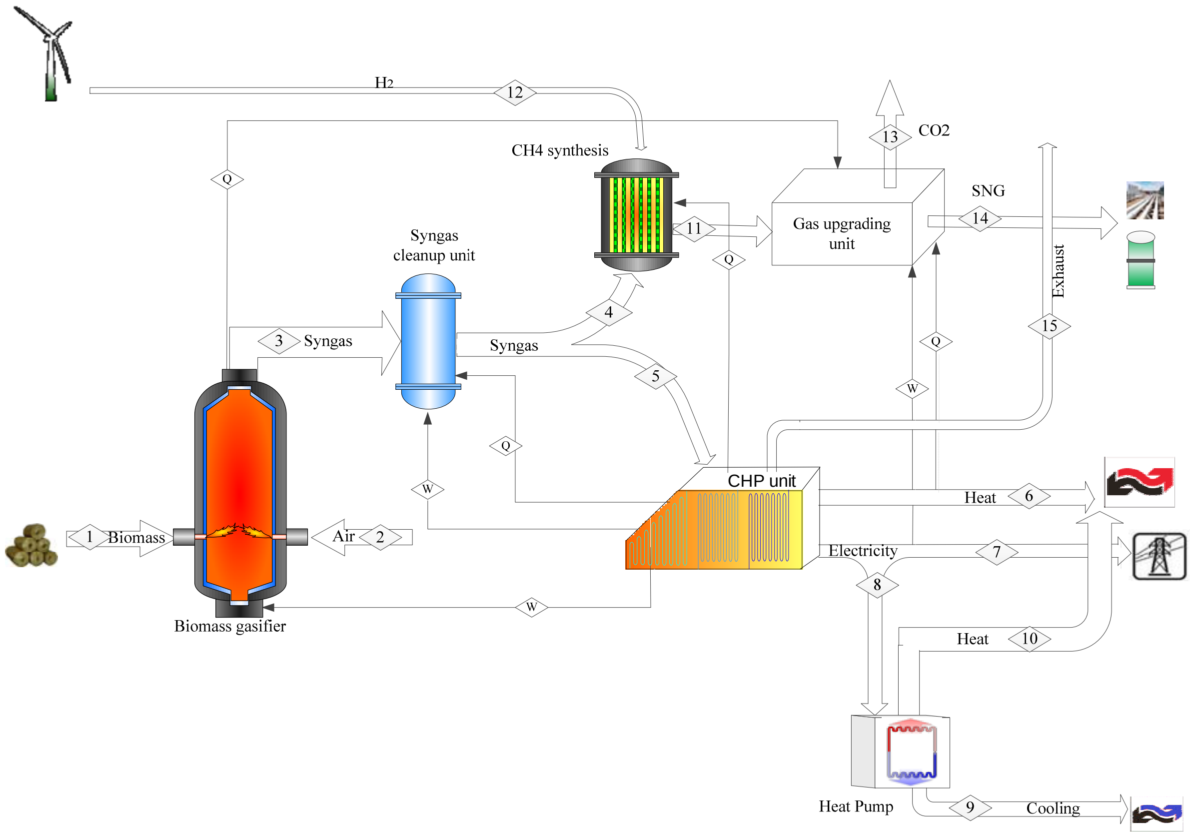


Fig.2 Simplified scheme of the proposed quad-generation system

H_2:CO ratio for methane synthesis. In the water-gas shift reaction, COand H_2O are converted to CO_2 and H_2.

5. In the methanation reactor, CO and H_2 are converted to CH_4 and H_2O in a fixed-bed catalytic reactor. Because methanation is a highly exothermic reaction, the increase in temperature is controlled by recycling the product gas or using a series of reactors. After gas upgrading, SNG is ready for applications.

As the heat demand varies during the year, there is a need for different case studies for the best utilization of total capacity. Therefore, the above system is designed for five cases based on output ratios.

- SNG-0: In this case, natural gas is replaced by bio-syngas and the gasification unit, with100% of the syngas used to generate power, heat and cooling and 95% of the CO converted first to CO_2, which is used in the combined cycle.

- QUAD-75:In this scenario,75 % of the bio-syngas is converted to generate power, heat and cooling and25 % of the syngas is converted to H_2-rich gas is used in methane synthesis for SNG production.

used to generate power, heat and cooling, and the other 50% of the syngas is converted to H_2-rich gas to be used in methane synthesis for SNG production.

- QUAD-25: In this case, 25 % of the bio-syngas is used for power, heat and cooling generation and75 % of the syngas is converted to H_2-rich gas to be used in methane synthesis for SNG production.

- SNG-100: All of the syngas is used in methane synthesis for SNG production.

IV. Model Description

The ASPEN PLUS process simulation software is used to model the systems evaluated in this paper. It offers a variety of thermodynamic property methods for process simulations. Some investigations conducted on biomass gasification (Wang, 2009; Doherty, 2010; Nikoo Mehrdokht, 2008) have shown that ASPEN PLUS is capable of predicting performance under diverse operating conditions. The Peng Robinson equation of state with the Boston-Mathias alpha function (PR-BM) has been used to estimate all of the physical properties of the conventional components in the gasification process (ASPEN Technology, 2010; Ramzan, 2011). The alpha parameter in this property package is a temperature dependent variable that improves the correlation of the pure component vapor pressure at very high temperatures. For this reason, this property package is suitable for simulating gasification processes that involve fairly high temperatures. 'HCOALGEN' and 'DCOALIGT' are selected for the enthalpy and density property models, respectively, for both biomass and ash.

Regarding the process simulation, the following assumptions have been made:

1. process is in steady state and isothermal.

Table 1. Process design parameter assumptions for simulation

Item	Unit	Value
Gasification unit		
Temperature	°C	1100
Pressure	bar	25
Air for gasification	t/h	96
Gas cleanup unit		
CO_2 removal	%	95
Sulphur removal	%	95
Electricity (Lv, 2004)	kJ/mol (CO2 + H_2S)	1.9
Steam (Lv, 2004)	kg/mol (CO2 + H_2S)	6.97
Power, heat and cooling unit		
Gas engine inlet temperature	°C	650
Gas engine inlet pressure	°C	25
Air for gas engine	t/h	100
Isentropic efficiency of expanders	%	90
Isentropic efficiency of main compressors	%	88
Mechanical efficiency main compressor	%	98
Recycled water for heating	kg/h	2000
Recycled water for cooling	kg/h	1000
SNG synthesis unit		
SNG synthesis temperature	°C	270
SNG synthesis pressure	bar	20

2. This process is made-up to occur instantaneously at equilibrium with volatile products mostly made of H_2, CO, CO_2, H_2O, CH_4, and C_2H_4 (Lv,2004; Buekens, 1985).
3. The electricity and steam for gas cleanup unit is extracted from gas engine (CHP unit).

The process design parameter assumptions for the simulation are summarized in Table 1. The overall process is divided into different sections, which are described below.

A. Biomass Drying

Note that the Biomass is specified as a non-conventional component in ASPEN PLUS and is defined in the simulation model using the ultimate and proximate analysis. Part of the moisture portion of the non-conventional component representing the biomass materials (Table 2) in ASPEN PLUS is converted to conventional liquid H_2O in a stoichiometric reaction (RSTOIC) block. Air (1.01 bars, 60°C, 50% relative humidity) is pumped into the dryer. The water is evaporated in a countercurrent heat exchanger block using the process steam as a heat source. A small heat loss is modeled in the condensate return line and is assumed to be 2% of the dryer thermal load. A FLASH2 block is used to separate the exhaust vapors from the biomass material, and dried product (DRYBIOM) exits the dryer with 10% moisture content.

Table 2: Biomass characteristics (Lasse, 2010).

Properties/Biomass	Unit	Straw
LHV	***MJ/kg***	***17.65***
Ultimate Analysis	DAF	
C		48.39
H		6.15
O		44.68
N		0.58
S		0.09
Cl		0.30
Proximate Analysis	DM	
VM		77.36
FC		19.25
Ash		5.58

DM: dry matter; DAF:dry ash free

Table 3: Description of the reactor blocks utilized in the simulation

Block ID	Aspen floowsheet Name	Description
RYIELD	BIOMASS	Yield reactor-converts non-conventional biomass to conventional components by using FORTAN statement
RSTOIC	DCOMBIOM	Specify operating conditions, reactions, reference conditions for heat of reaction calculations, product and reactant components for selectivity calculations
MIXTER	MIXTER	Mix of air and decomposed biomass feed from DCOMBIOM and feed to GASIFIER.
RGIBBS	GASIFIER	Specify reactor operating conditions and phases to consider in equilibrium calculations
SEPRATOR	SEPRATOR	Separates gases from ash by specifying split faction.

B. Gasification Unit

Fig. 3 shows processes diagram for gasification unit. 'DRYBIOM' from the drying unit enters the 'BIOMASS'

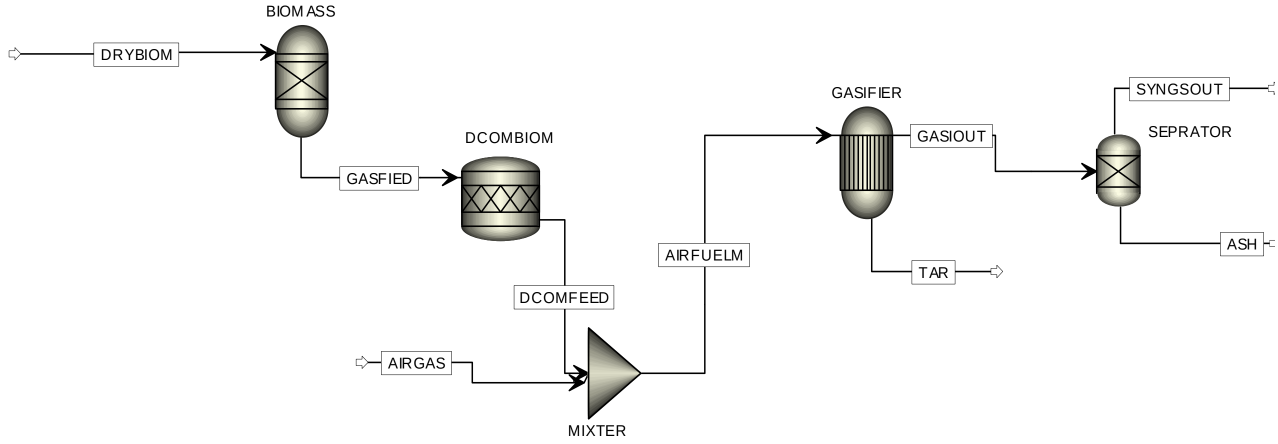


Fig.3 ASPEN PLUS model for the gasification unit

block at near-atmospheric pressure and the component yield of this block has to specify. It moves through an equilibrium reactor ‘DCOMBIOM’ and mix of air in a ‘MIXTER’. The stream continues to a RGIBBS block. It separates tar components from the stream. A description of the different ASPEN PLUS reactor blocks are given in Table 3. Raw syngas is produced from ‘GASIFIER’ with temperature 1100 ^{o}C and 25 bar. Then, the ash is separated from the syngas and flow into cleanup unit. The gasification reactions occur in (‘DCOMBIOM’) according to the reaction set shown in below.

$$C + 0.5O_2 \rightarrow CO \quad (1)$$

$$C + CO_2 \rightarrow 2CO \quad (2)$$

$$C + H_2O \rightarrow CO + H_2 \quad (3)$$

$$C + 2H_2 \rightarrow CH_4 \quad (4)$$

$$CO + 0.5O_2 \rightarrow CO_2 \quad (5)$$

$$H_2 + 0.5O_2 \rightarrow H_2O \quad (6)$$

$$CO + H_2O \rightarrow CO_2 + H_2 \quad (7)$$

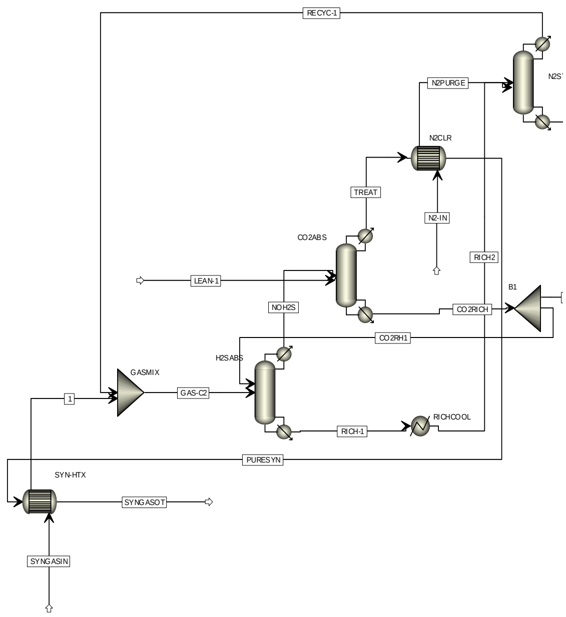
$$CH_4 + H_2O \rightarrow CO + 3H_2 \quad (8)$$

$$H_2 + S \rightarrow H_2S \quad (9)$$

$$0.5N_2 + 1.5H_2 \rightarrow NH_3 \quad (10)$$

C. Gas cleanup unit

After the synthesis gas leaves the gasifier, it must be processed for further use. First, the synthesis gas passes through a gas cooling heat exchanger block, ‘SYN-HTX’, which generates process steam. The gasification of these biomass fuels will produce components such as H_2S, and NH_3, which can be harmful to equipment and produce pollutants during synthesis gas combustion. Next, the gas passes through a wet scrubber, ‘H2SABS’, to remove sulfur matter. After that the stream



continues to block ‘CO2ABS’ where it can produce ‘CO2RICH’stream and $CO_2$is separated through block ‘B1’.The next stage in gas processing is the selective removal of harmful components through ‘N2STRP’ block (Fig.4).

D. Power, heat and cooling production unit

Clean syngas from the gas clean-up section enters the gas engine, where it combusts in ‘COMBA’ (Fig. 5). The stream continues into an expander ('EXPN1') and burns in a reactor ('BURN')in the presence of air. The flue gas is used to run 'EXPN2'and 'EXPN3'. The total work from all the 'EXPN's are combined in 'WORKMIX' and are split (80:20) again into two streams, with 20 % of the produced power used for the cooling system and the exhaust gas from 'EXPN3' used for district heating purposes. District heating water from the users (make-up water) returns as 'DHWIN1' and 'DHWIN2' and is heated by heat exchangers ('B3'and'B2'). Both 'DHWOUT1' and 'DHWOUT2' outputs from the heat exchangers are utilized for the district heating system.

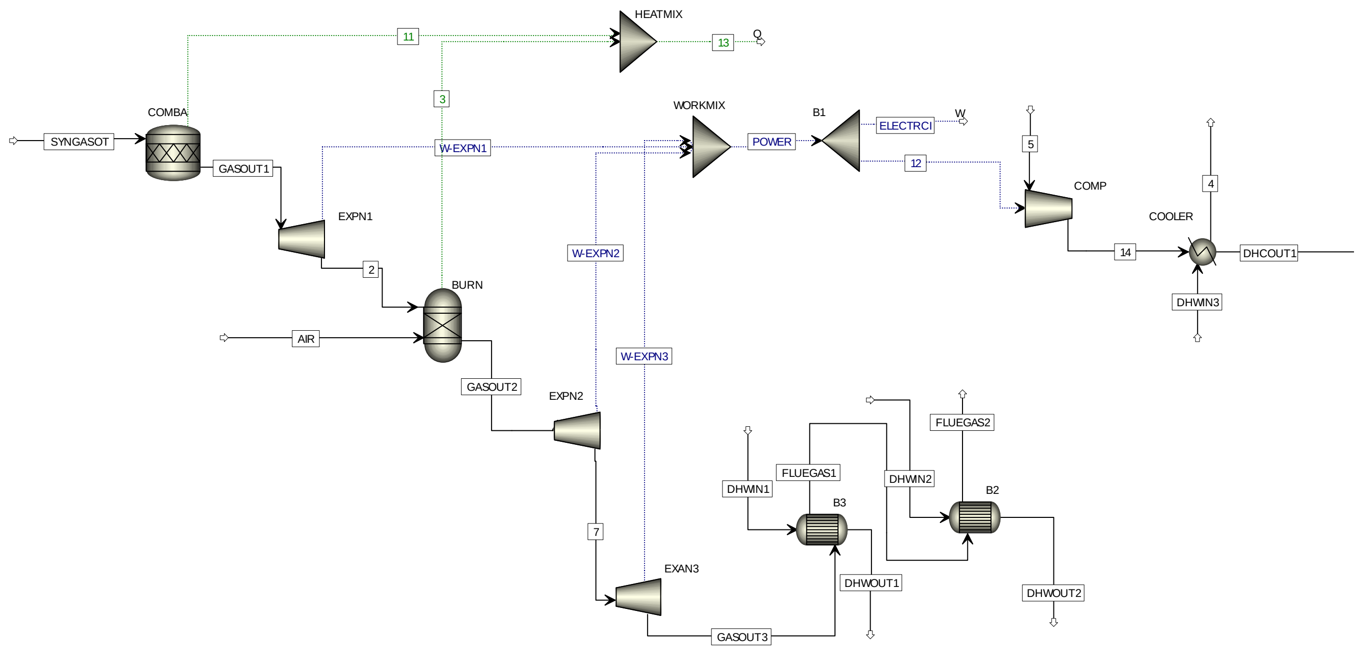


Fig.5 Power, heat and cooling production model

E. SNG production unit

The 'SYNGASOT' stream leaves the gas cleanup mix with additional hydrogen 'H2IN' in the 'MIXTER' block and continues to the methanation reactor, 'METHANT'. Additional, H_2 feed is necessary to provide CO/H_2 ratio. Fig. 6 shows the CH_4 synthesis process. In the methanation reactor, CO and H_2 are converted to CH_4 and H_2O in a fixed-bed catalytic reactor.

$$CO + 3H_2 \rightarrow H_2O + CH_4 \quad (11)$$

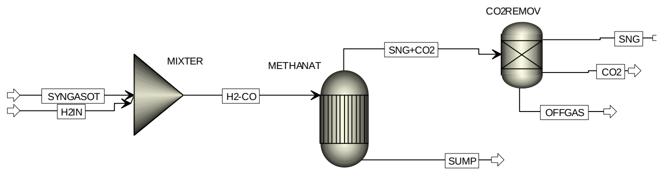


Fig.6 SNG synthesis process

The produced CH_4 still has some impurities, so it enters a separator unit, 'CO2REMOV', where the CH_4 is separated from CO_2.

F. Sysem evaluation criteria

The net energy efficiency (NEE) of the quad-generation system can be defined as (Ahrenfeldt, 2012, Wang, 2009):

$$\eta = \frac{\sum E_{products}}{\sum E_{feedstocks}} \quad (12)$$

$$= \frac{E_P}{E_{in}} + \frac{E_H}{E_{in}} + \frac{E_C}{E_{in}} + \frac{E_{SNG}}{E_{in} + E_{inH_2}} \quad (13)$$

$$= \frac{E_P}{E_{in}} + \frac{E_H}{E_{in}} + \frac{E_C}{E_{in}} + \frac{E_{SNG}}{E_{in} + E_{inH_2}} \quad (14)$$

Where E_P, E_H, E_C and E_{SNG} are the output energies from power generation, heat production, cooling energy and the SNG process, respectively. E_{in} represents the total energy input to this quad generation plant which includes power and heat input during gas cleanup unit, and E_{in,H_2} is the hydrogen energy input to the SNG synthesis process. η is the net energy efficiency, and η_P, η_H, η_C and η_{SNG} are the power, heat, cooling and SNG efficiencies, respectively. The efficiency is calculated on the basis of the lower heating value (LHV).

V. RESULTS AND DISCUSSION

The detailed energy consumptions for a quad-generation plant are shown in Table 4. For 100 tons per day of biomass input, SNG-0 utilizes 7625 kg/h syngas for power, heat and cooling production, while QUAD-25 uses 2287.5 kg/h for power, heat, and cooling production and 5337.5 kg/h for SNG production. The necessary amount of air for power production is reduced from SNG-0 to QUAD-25, as this case produces less electric power from the gas engine. The amounts of H_2 necessary for CH_4 synthesis are 66.24, 52.41, 42.31 and 35.76 kg/h for SNG-100, QUAD-25, QUAD-50 and QUAD-75, respectively, which are equivalent to 2.23 MW, 1.76 MW, 1.41 MW and 1.2 MW and it is presented by the LHV of H_2. H_2 is generated from an external source,but the increase of H_2 does not compensate for the energy loss that results from the smaller amount of carbon (C) in the syngas for CH_4 synthesis. Additionally, the flow rate of make-up water is 3 tons/h for each case.The SNG-100case has the highest CO_2 capture ability mainly because of its maximum ability to convert CO to CO_2. This results in the most energy loss and the lowest percentage of CO_2 emissions in the exhaust.

Fig.7 shows the energy balance for the quad-generation system. It also indicates the amounts of the four outputs from the SNG-0, QUAD-75, QUAD-50, QUAD-25, and SNG-100 cases. It should be noted that the amount of syngas produced from the gasifier has been kept constant for all of the cases. According to the different amounts of syngas utilization, this process produces approximately 49.728, 73.595, 95.22 and 134.34 m^3/h of SNG forthe QUAD-75, QUAD-50, QUAD-25 and SNG-100 cases, respectively. Simultaneously, it generates 11.1, 8.6, 6 and 5 MW of heat in the SNG-0, QUAD-75, QUAD-50 and QUAD-25 cases, respectively. Twenty percent of the power generation from the quad-generation plant is used for the cooling system. The SNG-0 case does not produce any SNG, as all the syngas is used for power, heat and cooling production.

The primary measure of energy efficiency for a power plant is the feedstock to net power production ratio, but because the waste heat generated in the quad-generation plant is used for heat production, cooling, and SNG production, this measure is not an accurate representation of the efficiency of quad-generation plants. In this case, the net energy efficiency also includes the efficiency of the biomass used by all of the individual outputs. In Fig 8, the entire individual energy efficiency factor for the quad-generation plant can be observed. It also shows that the power efficiency for SNG-0 is 22.5%, while the efficiency for QUAD-25 is 6.9%, which is relatively low as it uses less syngas for power production. In the case of heat utilization, heat production efficiency is higher than the other output efficiencies. The heat production efficiencies are 24.47%, 29.37%, 42.1% and 54.34% for QUAD-25, QUAD-50, QUAD-75 and SNG-0, respectively. Fig. 8 also shows the cooling efficiency, which is the least efficient for all the cases, as it produces a smaller proportion of cooling relative to the total output. For SNG production, the efficiency increases gradually from QUAD-75 to SNG-100.For the SNG-100 case, fig. 8 does not show the power, heat and cooling efficiency as there is no production for this case. Similarly, fig. 8 does not include the SNG efficiency for the SNG-0 case.

Table 4: The material balance, power, heat, cooling and SNG produced, and utilities of five cases

Item	Unit	SNG-100	QUAD-75	QUAD-50	QUAD-25	QUAD-0
Feed stocks						
Biomass	t/day	100	100	100	100	100
Syngas for Power, heat and cooling	kg/h	7625	5718.75	3812.5	1906.25	0
Syngas for SNG	kg/h	0	1906.25	3812.5	5718.75	7625
Air for gasification	t/h	96	96	96	96	96
Air for gas engine	t/h	100	80	60	40	0
Make up water	t/h	3	3	3	3	3
H_2 input	kg/h	0	36.76	42.23	52.41	66.24
Waste Product						
Ash	kg/h	138	138	138	138	138
CO_2 capture during gas cleanup	kg/h	326.98	326.98	326.98	326.98	326.98
CO_2 capture during SNG production	kg/h	0	131.78	156.23	182.56	204.68

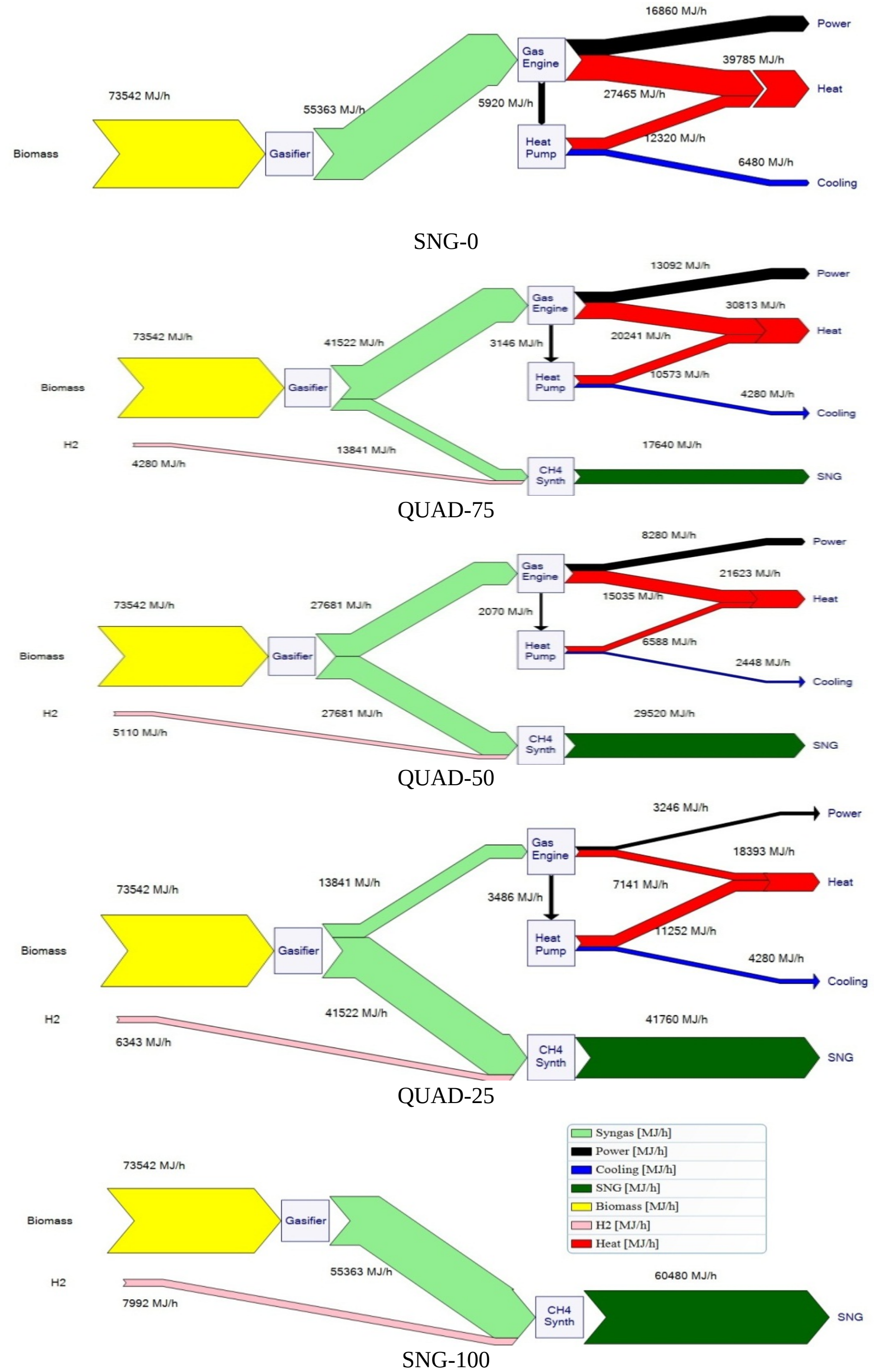


Fig. 7: Energy balances of the SNG-0, QUAD-75, QUAD-50, QUAD-25 and SNG-100cases for one hour of operation.

Temperature, pressure, mass and mole flows of different streams are listed in table 5 which refers to the numbers used the process diagram (fig. 2).The data from QUAD-50 case has reflected in this table. For an input of 4167.67 kg/hr of straw input, 657.35 kg/hr of SNG can be produced. Stream 1, biomass composition is analyzed in table 2. Stream 3, syngas has more mole components like H_2S, NH3, S and the values are 14.15, 31.73, 0.29 kmol/hr respectively. Stream7 and 8 represents the electricity to the grid and heat pump respectively.

Table 5: Parameters of the main points of the quad-generation system

Stream	Temperatur (°C)	Presure (bar)	Mass flow (kg/h)	Mole flow (kmol/h)								
				N_2	O_2	CO	H_2	CO_2	H_2S	CH_4	H_2O	C_2H_4
1	25	1.01	4167.67	-	-	-	-	-	-	-	-	-
2	25	1.01	1000	32	96.01	-	-	-	-	-	-	-
3	1205.01	28	7209.68	32.66	98.24	16.84	86.87	16.84	14.14	21.7	59.04	0.4
4	650	25	7625	-	10.2	19.35	56.66	0.84	0.71	18.66	41.02	0.4
5	650	25	3812.5	-	10.2	19.35	56.66	0.84	0.71	18.66	41.02	0.4
6	90	1.01	2000	-	-	-	-	-	-	-	55.51	-
7	-	-	-	-	-	-	-	-	-	-	-	-
8	-	-	-	-	-	-	-	-	-	-	-	-
9	5	1.01	362.32	-	-	-	-	-	-	-	55.35	-
10	95	1.01	502.72	-	-	-	-	-	-	-	15.6	-

The net energy efficiency (NEE) of four different cases is presented in fig.8. It can be observed that with increasing SNG production, NEE also increases. The lower NEE is also a result of transforming chemical energy into thermal energy, which is poorly converted to electrical energy, instead of transferring chemical energy to electrical energy. This means that the larger

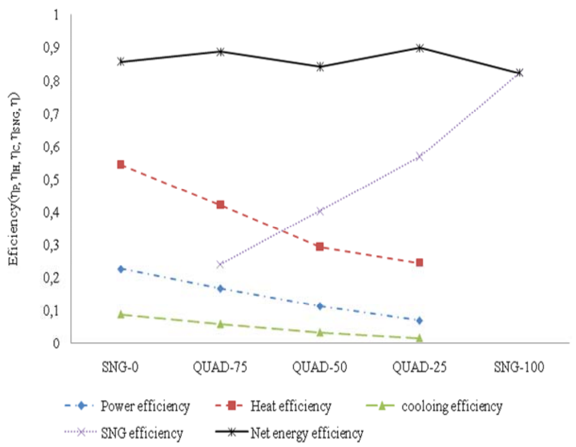


Fig. 8 Power, heat, cooling and SNG efficiencies for five cases

the power production shares, the lower the efficiency will be

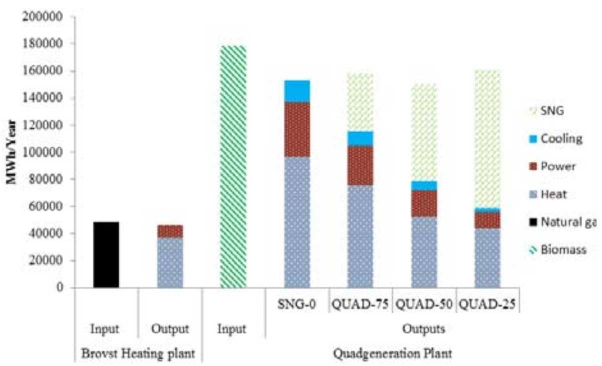


Fig. 9 Comparison of a quad-generation plant to an existing district heating plant

with respect to SNG production. The NEE for SNG-100 is relatively low as it captures the highest amount of CO_2 of all the cases.

Fig. 9 shows a complete comparison of the input and output products of a quad-generation plant and the Brovst DHP. In case of more heat production from quad-generation plant, it may serve the nearby localities as the municipality considered a joint distribution and production network. As described in the scope of the research, it is possible to utilize the maximum capacity of the plant by selecting different case studies and reducing the gap between the production and capacity curves.

VI. Conclusions

The quad-generation processes for the production of power, heating, cooling and SNG were modeled and compared in terms of design and energy efficiency analysis. The SNG-0 case is more appropriate for the winter as the demand for heating rises in this season, while the QUAD-25case would be more appropriate in the summer because it can produce more SNG and still produce some power, heat and cooling. In the case of excess power production from wind and a lower price for heat from other heating plants, SNG-100 would be a good option for a quad-generation plant. One of the advantages of this design is that the plant authority does not need to build storage for SNG as they already have access to the national natural gas grid. In this context, a process that converts biomass into SNG, which is equal in quality to fossil-derived natural gas, has been investigated. Such a product could easily be injected into the national gas grid to benefit from the existing distribution network for transport applications. With the increasing market share of gas engines in the transport sector, fossil fuels could therefore be partially substituted by a renewable fuel that is neutral in greenhouse gas emissions.

As the Danish Government aims to derive more of its energy from renewable fuels, this type of integrated quad-generation approach could be applied for any of the heating plants in other municipalities. This modeling approach can be used by other investigators who aim to change their operation strategies and plant designs from fossil fuel-based to renewable resource-based energy systems.

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Paper 2

Planning of a Quadgeneration power plant for Jammerbugt energy system.

Rudra, S.; Rosendahl, L; Hoffmann, J.

Proceedings of the 2nd European Conference on Polygeneration.

Planning of a Quad-generation power plant for Jammerbugt energy system

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Abstract

Quad-generation is the simultaneous production of power, heat and cooling and different fuels from flexible feedstocks such as biomass, waste, refinery residue etc. In order to accommodate more renewable energy into the energy system, it is extremely necessary to develop new flexible power plants that can quickly increase or decrease the production of electricity. Such plants should be ultra-flexible in terms of production and able to run on many different types of fuels, with one of its major outputs being liquid fuels for the transport sector. The aim of this paper is to integrate district heating energy technology into a Quad-generation energy system at Jammerbugt municipality in the north of Denmark in a creative and innovative manner that can reduce CO_2 emission and fuel limitations, whilst not compromising security of delivering heat and power to the local resident. So, it is essential to think about the design and co-optimization of energy system in this area. ASPEN Plus is used for process integration, where energyPRO is suitable for the investment planning and economic analysis. And also some CFD (Computational fluid dynamics) simulations shall have done for correct measurement of some equipments in the Quad-generation power plant. This paper presents two models for the investment planning of a Quad-generation energy system in Jammerbugt municipality, and uses these models for different case studies addressing the system for production of heat, cooling, liquid fuels and electricity.

Keywords

Quadgeneration, Planning, Jammerbugt, Energy system.

Introduction

The Danish Government's policy is that Denmark must be a green sustainable society. The stabilization of the Danish primary energy supply over more than three decades shows that the ability to act as a society has been possible despite conflicts with representatives of the old technologies. In Denmark, the description of concrete technological alternatives and alternative energy plans has played an important role. Denmark should also be among those three countries in the world which increase their share of renewable energy the most up to 2020 [1]. At present the share of renewable energy is coming close to 20 per cent. From such point of departure, a scenario framework has been established in which the Danish system is converted to 100 percent Renewable Energy Sources (RES) in the year 2060 including reductions in space heating demands by 75 percent [2]. A technical report has published which identify the role of polygeneration on a European level and document the activities taking place in Europe [3]. Energinet.dk, the owner of the overall energy infrastructure in Denmark, has allocated almost DKK 29 million for a consortium that develops the ultra-flexible power plant of the future [4]. Energy is an essential factor required for the development of societies and countries, but at the same time it represents a problem for an appropriate sustainable development. Energy is required for developing whatever activity in whatever field (education, health, agriculture, food production, water supply, industry and so on) but its present utilization represents one of the most important sources of environmental pollution and greenhouse gas emissions. In 2004 the total primary energy supply of the world was 11059 Mtoe (Million Tons of Oil Equivalent), and 80.3% of this energy supply came from fossil fuels [5].

Innovation in power generation technologies for higher efficiency and lower emissions has never ceased over the decades: the Integrated Gasification Fuel cell (IGFC) power plant combines a gasifier, a fuel cell and a steam turbine cycle for power generation, not only delivering reliable performance but also increased efficiency [6]. Statistics show that industry, transport and residential sector are the main energy consumers. In this respect, polygeneration technologies, more developed in chemical [7] and energy processes [8] but clearly unexploited yet provide: Maximum energy usage as a consequence of increasing energy efficiency, reduction of unit cost of final products, reduction of environmental burden.

A number of scientific publications address the mathematical modelling and simulation of polygeneration energy systems. However, they either focus on the evaluation of new plants and technologies [9] on the configuration design of processes [10]. Research in large-scale investment planning with the existing plant for polygeneration energy systems has been limited, albeit clearly crucial for strategic policy-making in regions and countries. The concepts of polygeneration and energy integration have been described with various examples of systems [11].

This study is carried out to select the best plan among many possible alternatives, according to explicit economic objectives, and subject to quantified technical and environmental constraints that vary by region. It is also describing the future technological involvement of the future Quad-generation energy system in Jammerbugt region.

Present heating system

Jammerbugt is one of the eleven municipalities in the North Jutland region (Figure 1). It has twelve district heating plants. Figure 2 shows the thermal basis for the 12 district heating plants in this municipality and the primary fuels that have been used for these plants. The total heating base is 252,200 MWh/year, of which four major works (Fjerritslev Aabybro, Jetsmark and Brovst) account for 78% combined. Seven of the plants have natural gas as primary fuel, four of them have woodchips and a single (Vr. Hjermitslev) has biogas. The purpose of this paper is to incorporate a Quad-generation power plant with the existing district heating power plant in the Jammerbugt municipality.

Figure 1: Denmark with Jammerbugt located in the North.

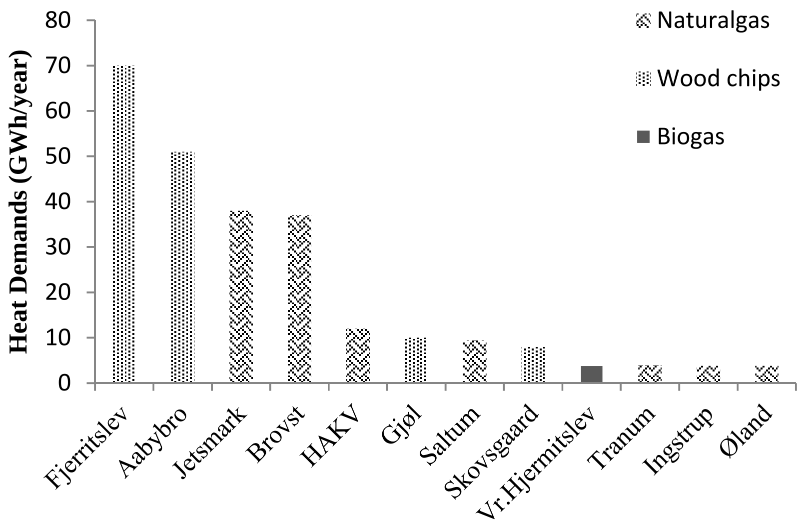

Figure 1: Heat demand and primary fuels for the 12 district heating plants in Jammerbugt municipality.

Scope of this Work

Jammerbugt municipality has a plan to combine all the decentralized heating plants to a district heating network. A plan for this region is to integrate all electricity, heating, cooling and transportation demands. Based on that scenario, it will be analysed to convert the possible district heating plant to Quad-generation plant which may helps to be 100 % renewable on the total energy system.

And also the use of fossil fuels is associated with a lot of concerns; among these the security of supply and air pollution associated with the combustion of fossil fuels – both local pollutants such as NO_x, SO_x and also CO_x. One of the ways of reducing the transportation sectors dependency on fossil fuels is by using biofuels from the Quad-generation plant. In this region, a large amount of electricity is being produced by wind frams but the output is always fluctuated according to the availability of wind. So this Quad-generation power plant can make room for those wind energy as it's possible to produce flexible output.

Modeling and simulation of Quad-generation system

A model of process simulation, CFD simulation and economic analysis will have been done towards design, investment planning and optimization of this Quad-generation system. Here an introduction for different softwares which we will use for our case evaluation has discussed.

ASPEN Plus:

The proposed Quad-generation process will be simulated using ASPEN Plus [12]. The ASPEN model of the Quad-generation plant consists of some individual sections: (1) CHP (combine heat and power) or gasification process, (2) Heat pump process, (3) Refinery synthesis process, and (4) the whole Quad-generation the power plant. All models of each part are built in the mechanism model. Based on the literature [6,13] and the data given by the different local district heating companies, a series of specified parameters for the process will be selected, while the thermodynamic properties (such as RK-SOVE, ELECNRTL, PR-BM) will be selected specifically for each process.

energyPRO :

energyPRO [14] is an input/output software tool which is used for modeling energy systems including polygeneration plant. Carrying out feasibility studies for Quad-generation plant is one of the most important steps in the decision-making process. energyPRO allows the user to carry out a comprehensive, integrated and detailed technical and financial analysis. A recent comparison [15] of the features of different software packages available in the market (for instance AEOLIUS, COMPOSE, EnergyPLAN, HOMER, INFORSE, TRNSYS16 and some custom build models) concludes that energyPRO is a powerful and flexible application. The main features and evaluation mechanisms of energyPRO are described briefly here.

energyPRO has three different modules: design, finance and accounts. The design module includes the design and optimization of a specific operation year. The finance module will allow the project to be evaluated over a number of years, and detailed cash flows can be obtained. The accounts module allows a deeper level of financial analysis (it includes taxes, depreciation and others).

energyPRO model calculates annual productions in steps of, typically, 1 h. The inputs are capacities, efficiencies and hour-by hour distributions of heat demand and electricity sales prices. The period of optimization is divided into calculation periods, where everything is constant, for example temperature, solar radiation, priorities, heat demand, electricity demand, cooling demand, production capacities and fuel deliveries.

ANSYS CFD:

Computational fluid dynamic (CFD) analysis [16] provides crucial insight of the different individual parts of power plant. It also presents the advanced geometry acquisition, mesh generation mesh optimization and post processing tools to meet the requirements for integrated mesh generation and post processing tools for today's sophisticated analysis.

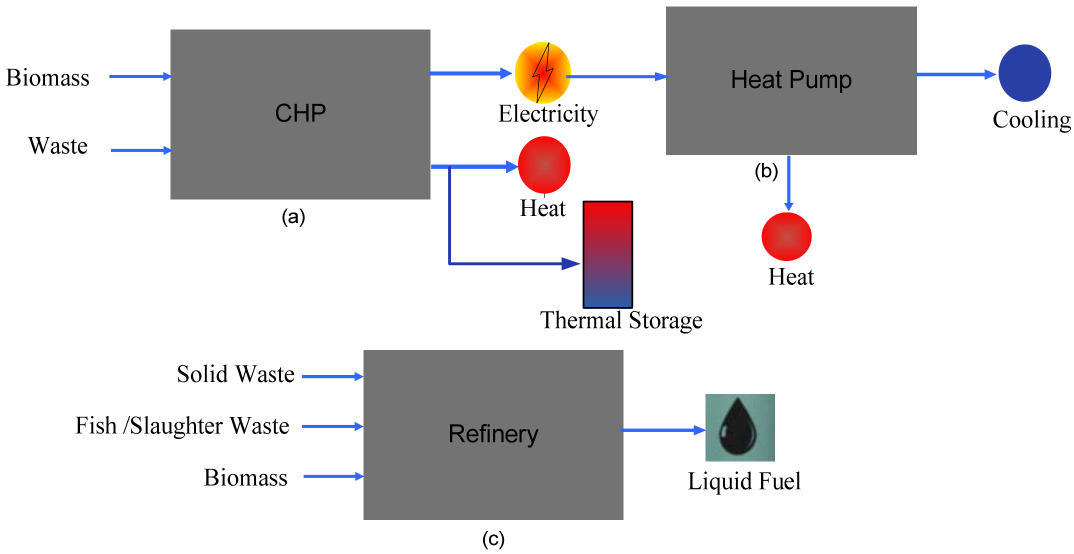

Figure 3: Quad-generation energy system with existing district heating plant.

Case studies and Results Discussion

Case 1: The case study using the model focuses on investment planning of Quad-generation energy systems with different productions (heat, cool, electricity and liquid fuels) at Jammerbugt in near future. Figure 3 illustrates the model for this case. The feedstocks which are available locally will be used in this power plant. For this case only heat pump and refinery equipments will attached in the existing district heating plant. Electricity produced from CHP (combine heat and power) plant will be utilized for the heat pump which will produce cooling for the end users. One additional part of refinery system will introduce here for the liquid fuel production (Figure 3). All the individual system will have stimulated by ASPEN Plus software. Besides the thermodynamic analysis, a techno-economic analysis of this system will also be done with energyPRO software which will help to establish this model in the economical point of view. And then system analyses will be verified by system simulations through economical point of views. This makes a highly flexible power plant that can run on a number of different fuels and produce electricity, heat, gas, or liquid fuels depending on what is required.

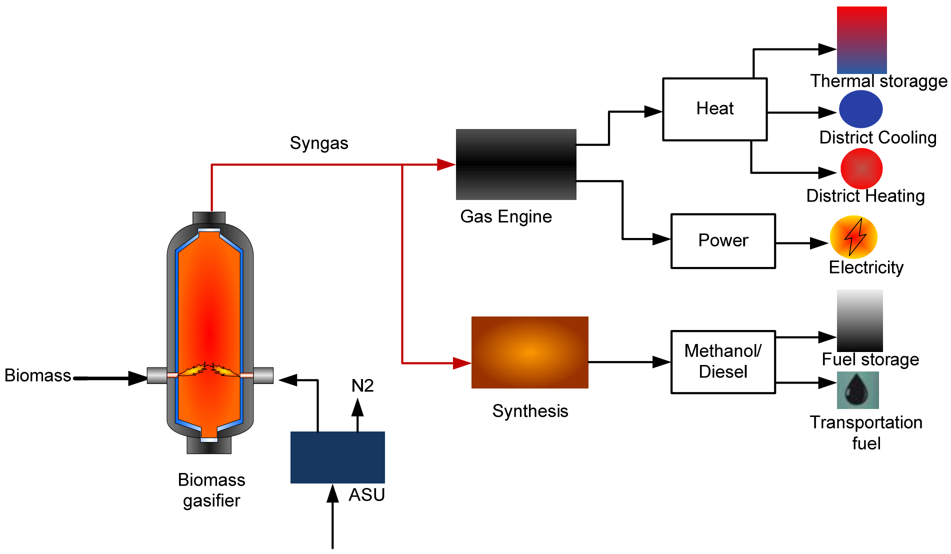

Figure 4: Quad-generation energy system with gasification unit.

Case 2: In this case, the Quad-generation plant consists of a gasification unit, where the primary fuels are converted to gas at high temperature by adding oxygen from air. The syngas consisting of CO and H_2 is then used for both the gas engine and synthesis unit which will convert the gas to methanol/DME under high pressure and after this, a distillation step separates the produced products. The gas engine will produce both heat and power which are used to the end users (Figure 4). It is also possible to introduce a heat pump which will use the power output from the gas engine and produce both district heating and cooling. This heat output can be utilized for district heating, district cooling and also for the storage purpose. The simulation for this model is also following the same procedure like case 1.

We will select some boundary conditions for the both cases of the Quad-generation system, and then simulate the different cases with the process simulator ASPEN Plus, CFD and energyPRO. The ASPEN Plus result sheet will be utilized for the CFD simulation for plant components. The spot market data which will be used for the energyPRO simulation will take from the Energinet.dk and also via Nord Pool's webpage. Mass flow and energy flow rates of each process which we will be obtained from the simulation results, will help to find out the way to improve the efficiency of the plant. For the environmental analysis energyPRO will measure how much of CO_2, SO_2 and NO_2 will emitted from the plant and its cost according to energy input of the system.

Superstructure based modelling strategy, along with ASPEN plus, energyPRO and CFD are efficient and effective in solving energy systems engineering problems, especially at decision making and planning stage. Based on this, multi-objective optimization and optimization under uncertainty produces further in-depth analyses and allows a decision maker to make the final decision from many aspects of view.

Conclusion

A Quad-generation energy system can improve profit margins and market penetration, decrease capital investment, reduce environmental emissions and increase feedstock flexibility crucially. Applications of this methodology to Quad-generation energy systems infrastructure planning problems will prove its superior ability to solve large-scale real industrial cases and its great potential to be more widely applied in energy systems engineering fields. According to the opinions of different plant owners, they are mostly interested into the Quad-generation system since it is possible to add some additional parts to their existing plant equipments. For this reason, case 1 having conventional combustion system might be preferable for this region instead of building new technology.

This study will find a way of planning to incorporate district heating energy technology into a Quad-generation energy system which can provide flexible outputs according to their needs that can reduce environmental emissions and fuel limitation.

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Paper 3

Optimization of a Local District Heating Plant Under Fuel Flexibility and Performance.

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OPTIMIZATION OF A LOCAL DISTRICT HEATING PLANT UNDER FUEL FLEXIBILITY AND PERFORMANCE

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ABSTRACT

Brovst is a small district in Denmark. Based on the case of Brovst, this paper analyses the role of district heating in future Renewable Energy Systems. The present use of fossil fuels in the Brovst DHP (district heating plant) represents an increasing environmental and climate-related load. So, an investigation has been made to reduce the use of fossil fuels for district heating system and make use of the local renewable resources (Biogas, Solar and Geothermal) for district heating purpose. In this article, the techno-economic assessment is achieved through the development of a suite of models that are combined to give cost and performance data for this district heating system. Different local fuels have been analyzed for different perspectives to find the way to optimize the whole integrated system in accordance with fuel availability and cost. This paper represents the energy system analysis mode energyPRO which has been used to analyses the integration of large scale energy system into the domestic drastic heating system. A model of the current work on the basis of information from the plant (using fossil fuel) is established and named as a reference model. Then different solutions are calculated for various local fuels in energyPRO. A comparison has been made between the reference model and the basis for individual solutions. The greatest reduction in heat price is obtained by replacing one engine with a new biogas where heat production is divided by 66% of biogas, 13% natural gas engines and 21% natural gas boilers.

INTRODUCTION

The Danish Government's policy is that Denmark must be a green sustainable society. The stabilization of the Danish primary energy supply over more than three decades shows that the ability to act as a society has been possible despite conflicts with representatives of the old technologies. In Denmark, the description of concrete technological alternatives and alternative energy plans has played an important role. Denmark should also be among those three countries in the world which increase their share of renewable energy the most up to 2020 (1). At present the share of renewable energy is coming close to 20 per cent. From such point of departure, a scenario framework has been established in which the Danish system is converted to 100 per cent Renewable Energy Sources (RES) in the year 2060 including reductions in space heating demands by 75 per cent (2). So, one of the steps for those aims is to optimize the decentralized district heating plant by reducing the fossil fuel uses and introduce locally available renewable resources as the primary fuel for those power plant.

A technical scenario has been described and developed for the transition of a Danish local energy supply from being predominantly fossil fuelled to being fuelled by locally available renewable energy sources. The scenario includes all aspects of energy demand in a local district i.e. electricity demands, heat demand, industrial demand as well as the energy demand for transportation (3). A study of Danish experience with methodologies and software tools has been done to design investment and operation strategies for almost all small CHP plants (4). The changes in such methodologies and tools in order to optimize performance in a market with fluctuating electricity prices have presented and discussed on that same paper. A simple linear programming model is presented to determine the optimal strategies that minimize the overall cost of energy for the CCHP (Combined cooling, heating and power) system. It has been shown that the optimal operation of this system was dependent upon load conditions to be satisfied (5).

Some of the studies have been done to reduce the combustion of fossil fuels and to introduce or expand the use of CHP by which the fuel efficiency in the system is improved (6-9). Primarily for environmental reasons, the Danish government subsidized the construction of cogeneration plants during the 1980s, even in small and medium scale applications (10), where most of them are using natural gas for their production.

Optimization of energy system is a key issue in the design of more sustainable development models. The Brovst DHP is optimized by using an optimization program called energyPRO that helps to decide the type of components and fuels used as well as the most profitable method of operating. Furthermore, it is desirable that the system is efficient and environmental friendly. The objective of this paper is to promote the most efficient and economic utilization of Brovst DHP and reduce the dependency on fossil fuels. In the present discussion, one can easily identify the efficient way of heat production according to fuel flexibility and economic consideration.

PRESENT HEATING SYSTEM

Brovst is one of the district heating plants in Jammerbugt municipality. Fig .1 shows the thermal basis for the 12 district heating plants in this Municipality and the primary fuels that have been used for these plants. The total heating base is 252,200 MWh/year, of which four major works (Fjerritslev Aabybro, Jetsmark and Brovst) account for 78% combined. Seven of the plants have natural gas as primary fuel, four of them have woodchips and a single (Vr. Hjermitslev) has biogas. Brovst plant only uses the natural gas for their production which heat demand is approximately 37200 MWhr/year (Fig.1). It is situated at Bøgebalke (Northern Denmark). At this present moment, it has 1285 customers on the network in Brovst who are both individual housing and industrial. Right now it has two generator sets with an output of 3.1 MW electricity and 4.1 MW of heat. Produced electricity is used for the internal demands of this plant. It also has two boilers where first one can produce 5 MW heat and another one 3.15 MW. Table 1 shows different units, primary fuels and their production rates. A 1600 m^3 storage tank has been installed in this plant. The efficiencies of boilers are more than 100% as they extracted additional heat from the flue gas. There is an emergency generator which can provide electricity if any accident will happen, so heat is maintained for all time.

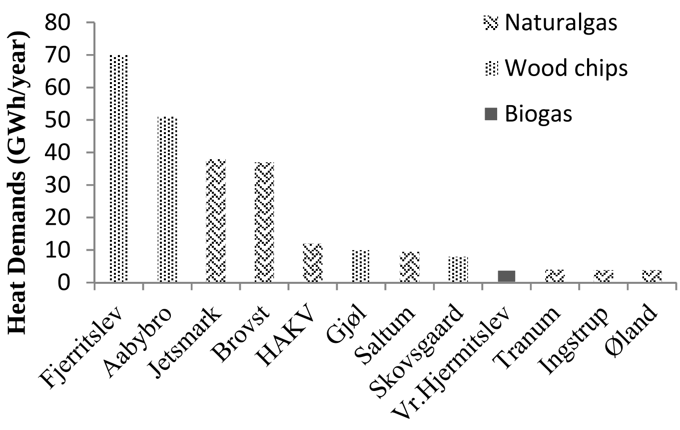

Fig.1: Heat demand and primary fuels for the 12 district heating plants in Jammerbugt municipality.

Table 1: Primary fuel, heat and power output of Brovst plant.

Unit	Fuel -	Thermal input KW	Heat Production(η) KW	Electricity Production(η) KW
Engine 1	Natural Gas	7654	4100(53.6%)	3100(40.5%)
Engine 2	Natural Gas	7654	4100(53.6%)	3100(40.5%)
Boiler 1-2	Natural Gas	7913	8150(103.0%)	-

METHOD

energyPRO COMPUTATIONAL PROCEDURE

energyPRO (11) is an input/output software tool which is used for modeling energy systems including district heating plant. Carrying out feasibility studies for district heating plant is one of the most important steps in the decision-making process. energyPRO allows the user to carry out a comprehensive, integrated and detailed technical and financial analysis. A recent comparison (12) of the features of different software packages available in the market (for instance AEOLIUS, COMPOSE, EnergyPLAN, HOMER, INFORSE, TRNSYS16 and some custom build models) concludes that energyPRO is a powerful and flexible application and is by far the most complete software in terms of modeling different scenarios. It allows prioritizing in terms of which production units operate first, which is an advanced capability that none of the similar software tools have. In Denmark, most small district heating and CHP plants have been designed using this computer tool (4). For the above reasons energyPRO has been chosen for the analysis in this present study. The main features and evaluation mechanisms of energyPRO are described here.

energyPRO has three different modules: design, finance and accounts. The design module includes the design and optimization of a specific operation year. The finance module will allow the project to be evaluated over a number of years, and detailed cash flows can be obtained. The accounts module allows a deeper level of financial analysis (it includes taxes, depreciation, spotmarket prices, etc). In all these modules, the user must define the demand profiles, the equipment, fuel and electricity tariffs, and the plant control strategy.

energyPRO model calculates annual productions in steps of, typically, 1 h. The inputs are capacities, efficiencies and hour-by hour distributions of heat demand and electricity sales prices. The period of optimization is divided into calculation periods, where everything is constant, for example temperature, solar radiation, priorities, heat demand, electricity demand, cooling demand, production capacities and fuel deliveries. The calculation periods can be divided into groups, typically groups in which the electricity prices are the same [4]. The traditional method of calculating energy production is to make chronological hour-by-hour calculations, trying to take into account that, for example, production during night hours may fill the thermal store too soon. This hinders more attractive production from being placed in the morning of the following day.

In contrast to the traditional chronological order approach, energyPRO places productions in the most favourable periods for a whole year. As a consequence, before being accepted, each new planned production is carefully checked so that it does not disturb already planned, more attractive future productions.

THE energyPRO MODEL

The model is an input/output model. General inputs are demands, capacities and the choice of a number of different regulation strategies, putting emphasis on import/export and surplus production of heat and electricity. Outputs are energy balances and resulting annual productions, fuel consumption and import/exports.

The different solutions are calculated in the program energyPRO. First a model of the current work on the basis of information from the plant has been established and this model is called the reference model. Reference model is then used as the basis for individual solutions. The energyPRO simulations have been done for biogas, solar, heat pump and Import case (heat from Aalborg). All the information that is required for energyPRO simulation is listed on the Annex .

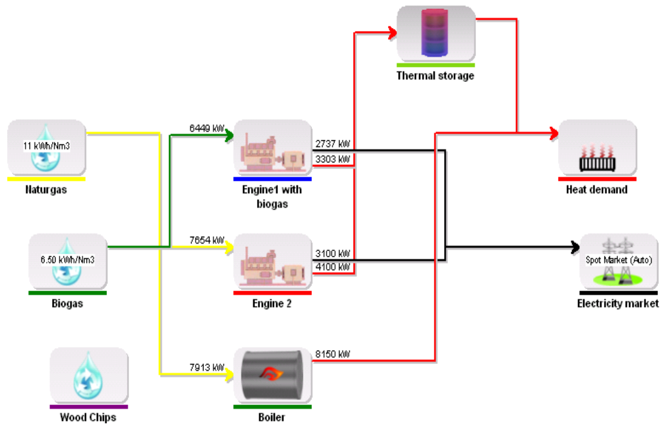

Fig. 2: energyPRO flowsheet for Biogas model

GENERAL REQUIREMENTS

The models in energyPRO are based on different assumptions. The general assumptions (for example energy prices) for these energyPRO simulations are contained in Annex. The plant-specific assumptions that have been informed by the work are also shown in the Annex. The set-up for the Brovst District plant is simple one with having two gas engines, two boilers and a heat storage tank of 1600 m^3.

The annual heat demand is 37 200 MWh and heating need is adjusted for differences between the number of days in the reported period and in a normal year.

Reference option:

For the reference model, only natural gas is used as a fuel for both engines and boiler. Natural gas consumption is 4,952,694.6 Nm^3. The model of the energy system and the applied operation strategy (user defined or auto calculated) determines the production and consumption of the production units. All data provided on the present heating section, table 2 and table 3, is also used as assumptions for the simulation of this reference option.

Biogas option:

For this option, the plant's one engine is replaced by a new engine (enbacher 620) with a power of 2737 KW_{el} that can run on both biogas and natural gas. Another engine and boiler use natural gas. Biogas and natural gas consumptions are respectively 5,437,003 Nm^3 and 407,749.5 $Nm^{3.}$ Heat value of biogas is 6.50 KWh/Nm^3.

Solar option:

The area for establishing solar thermal collectors is around 10,500 $m^{2.}$ The necessary data can be collected from the NCAR (National Center for Atmospheric Research) website. There are some 100 m transmission lines with the existing heat storage tank. This option also uses natural gas, consumption is 3,152,694.6 Nm^3 for the engines and boilers as all of them are active for heat and electricity production and the operating expenses are assumed as 0.8 €/MW. Investment for solar collector is based on the price curve from ARCON[a] (for solar collector between 500 m^2 and 20,000 m^2). One year's production from a solar heating system is required energy savings. The market price for energy is assumed to be 33.33 €/MWh. With an output of approximately 500 kWh/m^2/year, this gives a value of 16.67 €/m^2 which is equivalent to 6% of the investment. In the solar heating calculation, the values of the energy savings have been subtracted from the investment.

a. http://www.arcon.dk/

Heat pump option:

A compression heat pump of 5 MW_{heat} is established for heating purpose and must be considered in the energy conversion unit with others engines and boilers. The heat pump uses groundwater as a heat source. Reservations are made to obtain the necessary amount of groundwater in the plant area. In this option, natural gas consumption is 1,956,981Nm^3.

Import heat option (Heat from Aalborg):

There is one heat transmission pipeline of 40 km from Aalborg to Brovst. The capacity is 7.2 MW with a pipe dimension of DN (Diameter Nominal) 200. A DN 200 twin pipe Series 2 has a heat loss of 920 kW = 8,060 MWh / year. Total investment for heat exchangers, pumps and other accessories is around 0.067 million. The investment for transmission twin pipe per meter (Series 2) is represented by the following equation: 4 * Ø + 133.33 [€/m], where Ø is the pipe DN number and this formula is based on pipe prices from DN 100 to DN 450.

Economic analysis:

For economic optimization, this study introduces a simple method using the results from the simulation. Table 7 shows some of the components of cost estimates. The optimization of DHP in the previous options has been performed to meet the Danish triple tariff and the price setting in the Nord Pool electricity market [23]. In the simulation, it is also necessary to select market type according to electricity market section. The production costs are defined as the long term marginal costs of producing electricity on a combined cycle power station. Such costs include fuel, operation and maintenance costs and investment costs. The investment costs are adjusted by the net price index, and the fuel costs are adjusted according to international fuel prices. The rest of the parameters are fixed by the law. The main result from simulation is the annual operating result (excluding income from sales of heat). Net Heat Production Cost (NPC) is calculated by dividing operating costs by the produced heat. After investment needs of the individual solutions are estimated, the cost of capital (CC) will be projected. A good comparison between the solutions will be obtained by allocating capital cost of the produced heat. The sum of the NPC and CC is called GPC (Gross Production Cost). And the appropriate fuel will be selected from different fuel sources according to the net GP. Finally, the data will be used for further simulation on a large scale and combined into one system which will be more efficient according to performance, environment and cost.

RESULTS

The techno-economic optimization of the Brovst district heating plant in a competitive market is both a matter of investment design as well as operation performance. Operation performance should be considered in the initial designing of the plant including the size and number of DHP-units as well as possible heat storage facilities. To best utilize heat sale prices and optimize revenue calls depend on the engine capacity and heat storage facilities as well as the ability to start, stop and, maybe, part load DHP units.

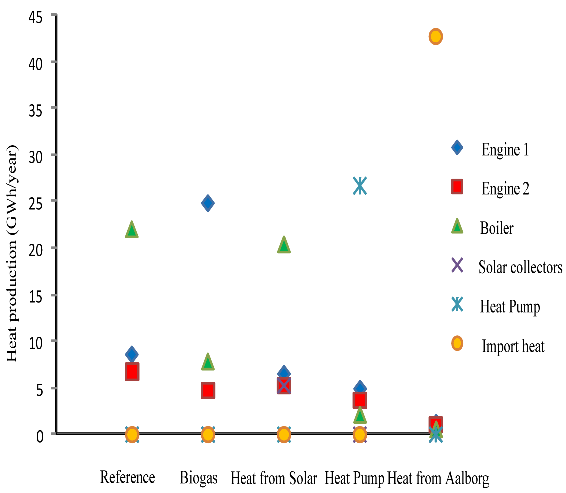

Fig. 3: The heat production according to different fuels.

All of the following identification of optimal Brovst heating plant's options are compared with the existing reference option consisting of natural gas engines and boilers. The comparison of heat production from engines and boilers for all the options are illustrated in fig.3. In the reference option, the heat is generated by natural gas, 41% by the engines and 59% by the boilers, respectively. For the Biogas option, engine 1 produced most of the heat (approximately 25000 MWh/year) as it uses both biogas and natural gas. This solution assumes that plant authority need to buy 7.4 million Nm^3 of biogas per year delivered to the plant. The financial benefit of this solution comes mainly from the subsidy for biogas based power generation at 0.054 € /kWh (1.11 million €/year). Heat production is produced by 66% of biogas, 13% natural gas engines and 21% natural gas boilers. The solar option proposal establishes a solar heating system of 10,500 m^2 which comes from an economic optimization point of view. More than 20000 MWh/year of heat is produced by the boiler from the 10,500 m^2 solar panel. The plant produces 5200 MWh per year, equivalent to an annual solar penetration of 14%. The remaining heat is produced from natural gas engines (31%) and boilers (55%). The Solar option leads to a reduction in heat price of 3.33 € /MWh. It has a relatively modest impact on heat cost due to limited sun coverage. The pump solution proposal establishes a groundwater heat pump based on 5 MW heat. The heat pump produces 72% of the heat and the remainder is produced with natural gas engines (23%) and boilers (5%). The solution proposed by heat from Aalborg establishes a 40 km long heat transmission line from Aalborg to Brovst. And in this case, Brovst has 42641.5 MWh/year (Fig. 3) of heat with the transmission loss is relatively higher than other options. The heat was purchased for 38.67 €/MWh, resulting in a total net generation price of 35.87 €/MWh. The solution was weighed down partly by the heat losses in the transmission line (22%) and partly by significant investment where the cost of capital is 20.93 €/MWh. In the heat pump option, 94% of the heat comes from Aalborg, 5% from natural gas engines and 1% from the boilers (Fig. 3). It should be mentioned that there is considerable uncertainty on the investment because the price of transmission lines is very flexible.

Fig. 4 shows that the amount of electricity produced from engine 1 is greater than that of engine 2 in all cases. For the biogas option, engine 1 has generated 20,499 MWh/year which is the highest electricity production similar to the previous heat production.

A thermal store is one way of solving this mismatch between the need for electricity and heat. The duration curve of heat demand and production from the all components for the Biogas option is shown in fig. 5, with the black single line expressing heat production. It shows that the production does not hour by hour match the demand. The reason is that a thermal store is displacing production in order to operate the plant more efficiently.

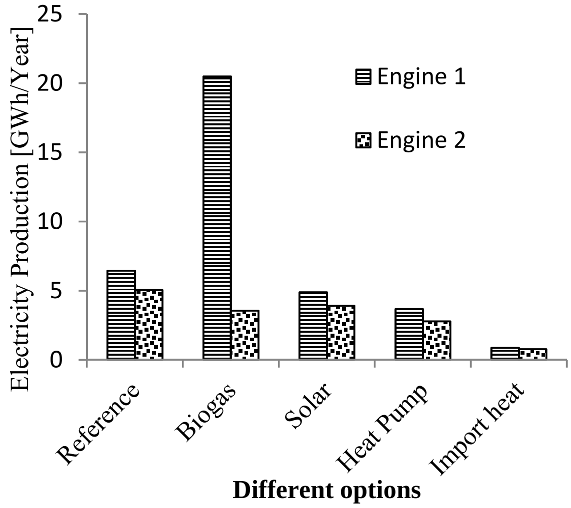

Fig. 4: The electricity production according to different fuels.

Fig. 5: Duration curve of heat demand and production.

The annual demand for and annual generation of 37,200 MWh for the Brovst District Heating results in operating expenses of 1.95 million €/year, equivalent to a net generation price (NPC) of 52.53 €/MWh. The investment cost for different options is shown in table 8, as well as a comparison of NPC, CC and GPC. In the case of import heat from Aalborg, total investment cost and capital cost are relatively higher than the other options.

Fig. 6 shows the different heat production price according to the fuel options. The best option for saving money is the Biogas option where it is possible to save 28.5 €/MWh considering the reference case as zero savings. To transfer heat from Aalborg to Brovst, takes almost 4.4 € /MWh more than the reference option. Though the price per MW heat is 0.67 € higher for the heat pump case, it is preferable to select this option rather than the solar option as it uses relatively less natural gas.

It is important to be aware that the actual prices can be both higher and lower than the calculated values. Also, the dimensioning of the individual solutions are based on qualified estimates, and therefore it is possible that further optimization of the proposals could result in lower heating rates than those presented in this paper.

Table 2: Economic evaluation of Brovst heating plant according to the fuel selection

	Brovst district heating plant	Invest ment	NPC	CC	GPC
	Unit	M €	€/MWh	€/MWh	€/MWh
0	Reference	0.0	52.53	0	52.53
1	Biogas	1.33	19.33	4.67	24
2	Solar	2.44	43.87	5.2	49.07
3	Heat Pump	2.53	39.73	8.8	48.53
4	Heat from Aalborg	9.73	35.87	20.93	56.8

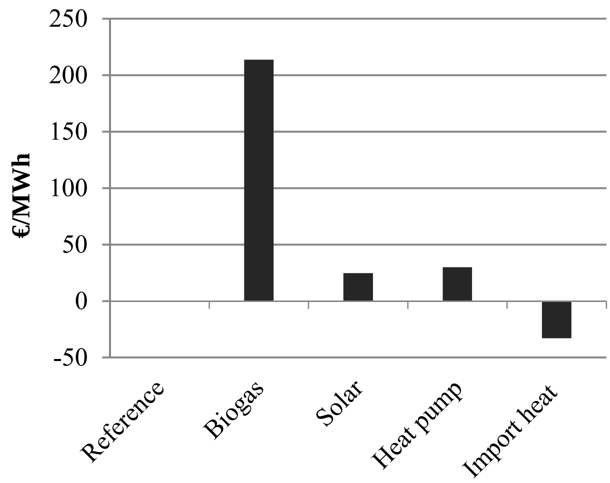

Fig. 6: Variation of heat production price according to different fuel options

CONCLUSIONS

Locally available renewable energy resources should be considered when an energy system is designed and analyzed by a systems analysis model, yielding results on an aggregate annual level as well as on an hourly basis. The purpose of the calculations presented in this paper has been to optimize the Brovst DHP according to reduction of heat production price. The different combinations are ordered to provide for a qualified basis to make a preliminary sorting of the suggestions. It shows the price of heat production for different options. By getting individual solutions from simulations, this study combines all the economic outcomes for making a decision regarding fuel selection and engine performance. This work concludes that the best solution is to combine a gradual expansion of the district heating production with the biogas option where 66% heat is produced by using biogas, 13% natural gas engines and 21% natural gas boilers. The next best option is the Heat pump option as it uses less fossil fuel than the solar option. Furthermore, this municipality considers a joint distribution and production of geothermal heat to be established as a municipal cooperation which may serve the nearby localities. It also helps to reduce the heat production from natural gas in Biogas option.

This conclusion is valid both in the present systems, which are mainly based on fossil fuels, as well as in a potential future system based on 100 % renewable energy. Since the fuel prices and other taxes are similar in the Jammerbugt municipality, this techno-economic optimization method could be applied for the other heating plants in that municipality. The modeling approach is also usable for other investigators who want to optimize operation strategies and plant designs. In that case, they only need to change the input data according to the actual conditions.

Acknowledgments

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ANNEX

Table A-1: Technical input for the simulation

The annual heat demand	37 200 MWh
Temperature of hot water supply	around 80˚ C (winter) around 75˚ C (summer)
Recycle water temperature	around 37˚ C (both summer and winter)
Storage water temperature	around 95˚ C
Heat storage tank capacity	1600 m^3
Natural gas fuel price	0.472 €/Nm^3
El-Spot	Time Values from 2008 (unweighted annual mean = 56.13 € / MWh)

Table A-2: Charges for emissions

Fuel tax	0.3 € /Nm^3 (2010)
CO_2 tax, engine	0.047 € /Nm^3 (2010)
NO_X-duty engine	0.0037 € /Nm^3 (2010)
CO_2 tax, boiler	1.573 € / GJ (2010)
CO_2 allowances	13.33 € / ton

Table A-3: Cost of rebuilding engine for biogas.

Biogas price	0.29 €/Nm^3
Reconstruction of Jenbacher Series 600	0.16 million €/piece
Reconstruction of Jenbacher Series 300 and 400	0.12 million €/piece
Miscellaneous:	0.067 million € / work

Table A-4: Heat pump investment including groundwater drilling

COP	2.5
Investment, heat pump	0.4 million € / MW_{heat}
Investment, drilling and others. (10%)	0.04 million € / MW_{heat}
Investment, power supply	0.05 million € / MW_{heat}
Investing, switching to work	0.067 million €
Operating expenses	1.33 € / MWh_{heat}

Table A-5: Heat loss of different pipes at 80 ° C/40 ° C

DN 80, 100, 125	13 W / m
DN 150	15 W / m
DN 200	23 W / m
DN 250	26 W / m
DN 300, 350, 400, 450, 500	35 W / m

Table A-6: General requirements of capital cost estimates

Inflation rate	2% per year
Depreciation Period:	
For transmission Cables, district heating, solar and heat pump	20 years
For Other investments	10 years
Loan:	
Interest rate	5% per annum
Maturity	As the amortization period
Performance	Inflation is not applicable for first year

Paper 4

QUAD-Generation: Techno-Economic Analysis Of A 100% Renewable Energy Plant For Flexible Local Production Of Electricity, Heating, Cooling, And Fuels.

Blarke, MB; Rudra, S.; Rosendahl, L

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QUAD-Generation: Techno-Economic Analysis Of A 100% Renewable Energy Energy Plant For Flexible Local Production Of Electricity, Heating, Cooling, And Fuels

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ABSTRACT

The character of local distributed energy systems is set to evolve from co-generation systems (electricity and heating), over tri-generation systems (electricity, heating, and cooling), to quad-generation systems (electricity, heating, cooling, and liquid or gaseous fuels).

Thereby, a single integrated state-of-the-art distributed energy plant may come to provide for all local energy residential, commercial, industrial energy demands, including transportation fuels.

An innovative quad-generation concept is presented, an operational dispatch model is developed, optimized using mixed-integer linear programming techniques, and analysed on an hourly basis with respect to techno-economic consequences, including energy balances, costs, and environmental impacts.

It is found that quad-generation provides a valid technological concept for complete 100 % renewable local energy systems that perfectly integrates multiple processes to supply local energy requirements, even the need for transportation fuels.

However, lifecycle costs are currently not competitive at projected fuel price levels.

Keywords: Quad-generation, renewable and distributed energy systems, gasification of biomass, large-scale heat pumps, techno-economic optimization.

1 INTRODUCTION

This paper evaluates a concept for Quad generation [1] by which a combination of electricity, some of which is self-generated, and biomass, here agricultural straw for energy, is converted to produce all four basic energy services: electricity, heat, cooling, and liquid or gaseous fuels.

While the Quad-concept could be admired for its ability to supply all basic energy services in island-mode, the concept could also support any national energy strategy for better integrating distributed energy producers. The concept is designed and operated to interact well with the surrounding energy system's markets and desire to balance intermittent renewables, such as wind power and solar energy. The concept will be established and operated to replace an existing natural gas fuelled combined heat and power plant in an energy system characterized by having an hourly spot market for electricity and high penetration rates of wind power.

The Quad-concept combines straw-fuelled gasification, syngas-fuelled engine and boiler, electrolyser and methane synthesis, compression heat pump, and thermal storages. It produces electricity, district heating and cooling, and synthetic natural gas (SNG). Electricity and SNG are traded in respective energy markets.

2 METHODOLOGY AND ASSUMPTIONS

The concept is modelled using COMPOSE [2, 3], which allows for techno-economic operational optimisation using mixed-integer linear programming (MILP) of complex cogeneration plants. The MILP program is formulated according to the standard formulation presented in Eq. (1):

$$\min \ f(x) = \sum_{\text{hour}=1}^{8760} \text{operational costs}_{\text{year, hour}} \quad (1)$$
$$s.t. \text{ linear constraints and bounds, and certain integrality constraints}$$

Thus, COMPOSE identifies the plant's optimal operational strategy by minimizing the economic cost of heat and cooling production for each year of operation under constraint of annual and hourly deterministic projections for energy requirements, O&M costs, unit capacities, and electricity and SNG markets. Fiscal costs are excluded and CO2 credits, if any, are not internalized. There is no capacity constraint on SNG sold and electricity sold/bought. A detailed description of the modelling framework and the operational optimization programming is provided in [4].

The plant is optimized for operation over a 20 year planning period from 2013-2032 under which it is stipulated that all investments are fully depreciated. The district heating requirements are based on historical requirements from an existing and typical distributed CHP plant with 1260 consumers [5], while the district cooling requirements are loosely estimated based on what could be the space cooling requirements of the area's commercial buildings. Projected annual fuel and electricity costs are based on official projections published by the Danish Energy Authority [6]. Investment costs and O&M costs are based on today's technology according to [7]. Table 1 to Table 4 present the key parameters that constitute the techno-economic constraints.

Table 1: Demand parameters.

Parameter	Annual [MWh/yr]	Annual projection	Hourly distribution
District heating requirements	37,200	Constant	According to Fig. 1D
District cooling requirements	5,000	Constant	Uniform (Fig. 1F)

Table 2: Fuel cost-benefit parameters. *Excludes trading costs and Public Service Obligations (PSO costs).

Parameter	Annual mean projection	Hourly distribution	Variable T&H/T&D
Straw cost	Fig. 1D	Uniform	€4.6 /MWh
Electricity spot market	Fig. 1C	Fig. 1B	€20.1 /MWh*
SNG market	Fig. 1E	Uniform	-

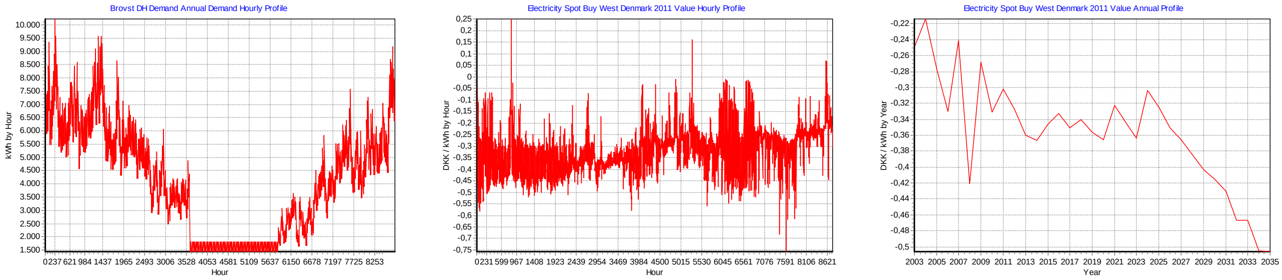
Table 3: Key design variables.

Existing CHP [5]	**Design capacities and conversion efficiencies**
CHP engine	8.2 MW-heat ($\eta_{\text{natural gas to electricity}}$=0.405, $\eta_{\text{natural gas to heat}}$=0.5357)
Heat-only condensing boiler	8.15 MW-heat ($\eta_{\text{syngas to heat}}$=1.03)
Hot thermal storage	1,600 m^3 (ΔT=50°), thermal heat losses to ambient location [8]

Quad-generation	**Design capacities and conversion efficiencies**
Existing CHP engine on syngas	6.6 MW-heat (25% lower, same efficiencies)
Existing boiler on syngas	7.5 MW-heat (25% lower, same efficiency)
Straw gasification unit	6 MW-fuel ($\eta_{\text{straw to syngas}}$=0.81, $\eta_{\text{straw to heat recovered}}$=0.10)
CH_4 synthesis and electrolyser	6 MW-fuel ($\eta_{\text{syngas-electricity to SNG}}$=0.86, 95/5 syngas-electricity ratio)
Cold thermal storage	1,600 m^3 (ΔT=20°), no thermal losses
Compression heat pump	1 MW-heat ($COP_{\text{electricity to heat}}$=2.5, $COP_{\text{electricity to cooling}}$=1.5)

Table 4: Key economic investment and operational cost parameters.

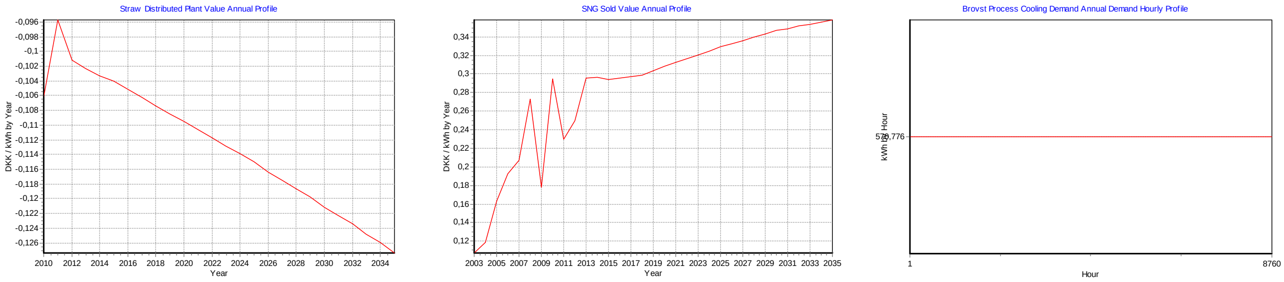
Parameter	Investment	Fixed operation	Variable operation
Existing CHP engine	-	-	€8.6 /MWh-electricity
Existing condensing heat-only boiler	-	-	€1.3 /MWh-heat
Straw gasification unit, CH_4 synthesis, electrolyser	€3.4M /MW-syngas	€78,000 /MW-syngas	-
Cold storage	€0.2M	-	-
Compression heat pump	€0.6M /MW-heat	-	€8.0 /MWh-heat



A. Projected hourly distribution of district heating requirements covering demand and grid losses.

B. Projected hourly distribution of electricity prices based on 2011 historical values.

C. Projected (from 2013) mean electricity spot market price.



D. Projected (from 2013) straw fuel cost excluding T&H costs

E. Projected (from 2013) SNG market value

F. Uniform hourly distribution of district cooling requirements covering demand and grid losses.

Fig. 1: Deterministic projected annual mean parameters and hourly parameter distributions. Exported from COMPOSE which bid that costs are negative values by convention thus resulting in falling curves when costs are increasing. Units in charts and text may differ.

3 RESULTS

Fig. 2 illustrates the Quad-concept's energy balance in 2013 optimized for least-cost operation. The overall direct fuel-to-energy efficiency is 97%. Straw consumption totals 64.9 GWh, or 16,000 tons of straw, corresponding to the annual output from 5,000 ha of agricultural land, corresponding to 0.2% of Denmark's farmed land in 2010. The plant sells 5 GWh electricity, purchases 1.8 GWh electricity, and sells 17.7 GWh SNG. The heat pump's share of total heat production is 16%, the CHP engine's share is 30%, while the heat-only boiler's share is 35%.

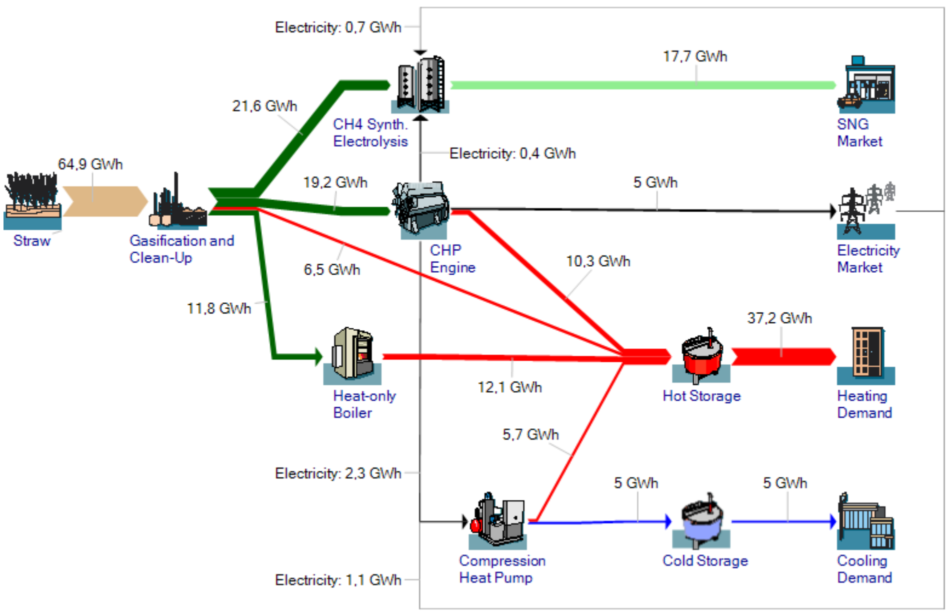
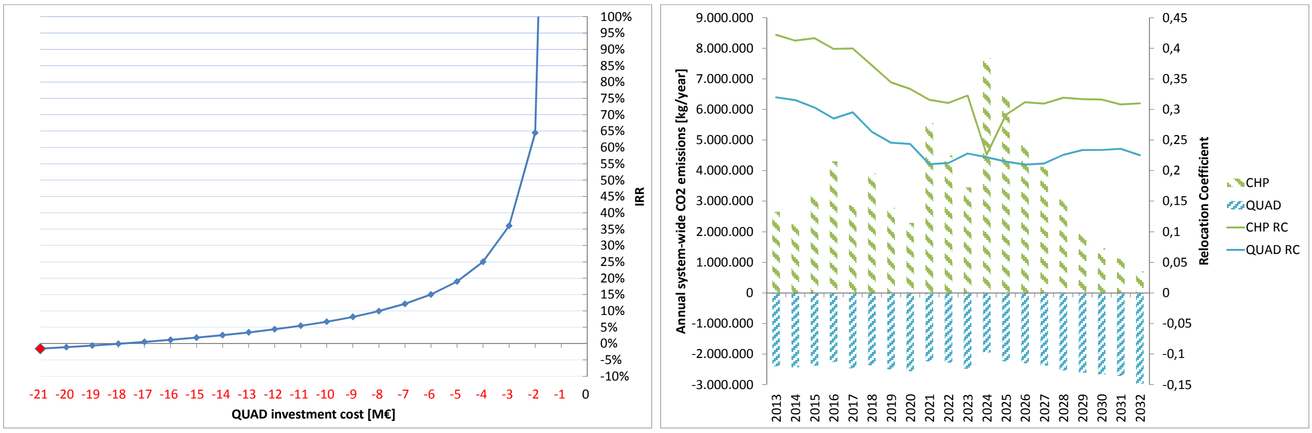


Fig. 2: 2013 energy balance of Quad-concept for optimal operation; straw-fuelled gasification with syngas engine and boiler, electrolyser and methane synthesis, compression heat pump, and thermal storages.

Fig. 3A shows that the base set of assumptions result in a negative economic internal rate of return (EIRR) of -1.6%. The EIRR break-even requires for the investment cost to be reduced by 16% compared to the base estimate given in Table 4, while an EIRR condition of 5% would require for the investment cost to be reduced by almost 46%. Fig. 3B shows that the system-wide CO2 emissions reduction declines from 9,638 ton per year in 2013 to 3,672 ton per year in 2032. In fact, the Quad-concept results in negative system-wide CO2 emissions as a result of the replaced natural gas from sold SNG and the replaced fossil fuel in central electricity generation from sold electricity. The annual variations are caused by the developments in fuel consumption and dispatch in central electricity generation, and the plant's operational dispatch, which also varies year by year due to fuel and electricity market developments.

Fig. 3B also compares the CHP and Quad operation by their "intermittency-friendliness" coefficient *Rc* for each year of operation. Blarke [9] has introduced the system-specific measure *Rc* for evaluating the intermittency-friendliness of an electricity producer or end-user. *Rc* is defined as the statistical correlation between the net electricity exchange between plant and grid, and the energy system's net electricity requirement. The net electricity requirement is defined as the electricity demand minus the intermittent electricity production. *Rc* serves to evaluate the marginal "goodness" of a plant's or end-user's response to variations in net electricity requirements ranging from -1.0 to 1.0.

It is found that *Rc* is *lower* for the Quad-concept, making it *less* intermittency-friendly, which is due to the Quad-concept's additional operational constraints. These constraints may be relaxed most cost-effectively by increasing the volume of thermal storages, secondarily by adding syngas storages, and increasing production capacities. However, such relaxations would result in higher investment costs without any significant change in net operational benefits, and thus jeopardize the economic feasibility.



A. Economic Internal rate of return (EIRR) and its sensitivity to investment costs (red point: base assumption).

B. Annual system-wide CO2 emissions and intermittency-friendliness *Rc*.

Fig. 3: Key results.

4 CONCLUSION

The paper investigates the techno-economic performance of an innovative straw-fuelled Quad-concept that produces all four basic energy services: electricity, heat, cooling, and liquid or gaseous fuels. This could be an attractive sustainable energy option for island-mode operation and for high-efficiency distributed generation systems.

It is found that Quad-generation offers significant CO_2 reductions and energy efficiency improvements, while the economic feasibility is jeopardized by high investment costs, which must be cut to almost half to achieve an EIRR of 5%. A CO_2 reduction cost of €138 per ton is significantly higher than today's low carbon credit prices in the European Trading System for carbon [10]. The poor economic performance does not currently favour Quad-generation in the energy system and markets considered in the investigation (West Denmark).

In terms of intermittency-friendliness coefficient *Rc*, both Quad-generation and reference CHP operation are hit by falling rates of "goodness". This is an important reminder that distributed generation is under pressure in energy systems with increasing penetration levels for intermittent renewables resulting in diminishing production rates – and increasingly so for complex systems such as Quad-generation.

Quad-generation's relatively lower intermittency-friendliness may be compensated by introducing syngas and hydrogen storages, increasing production capacities and increasing the volume of thermal storages. In the years ahead, such further advanced Quad-generation may provide a pathway for optimal co-existence between the biomass energy resource and intermittent renewables, such as wind power.

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Paper 5

Development of net energy ratio and emission factor for quad-generation pathways.

Rudra, S.; Rosendahl, L; Kumar, A.

Journal of Energy system, (Under review).

Development of net energy ratio and emission factor for quad-generation pathways

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Abstract*—The conversion of biomass to four different outputs via gasification is a renewable technology that could reduce the use of fossil fuels and greenhouse gas (GHG) emissions. This study investigates the energy aspects for a new concept of biomass based quad-generation plant producing Power, heat, methanol and methane. Circulating fluidized bed (CFB) gasifier and the gas technology institute (GTI) gasifier technologies are used for this quad-generation process. Two different biomass feedstocks are considered in this study. The net energy ratio (NRE) for six different pathways having the range of between 1.3–7.2.The lowest limit corresponds to the wood chips-based power, heat, methanol and methane production pathway using GTI technology. Since more efficient alternatives exist for the generation of heat and electricity from biomass, it is argued that syngas is best used for methanol production. The aim of this study was to evaluate the energy performance, reduce GHG and acid rain precursor emission, and use of biomass for different outputs based on demand. Finally, a sensitivity analysis is conducted for expected technological improvements and factors that could increase the energy performance.

Keywords*—*Net energy ratio, Quad-generation, Feedstocks, Syngas

I. INTRODUCTION

Biomass is a limited resource that needs to be used efficiently with low environmental impact, from extraction, conversion and distribution to end use. Biomass, including agricultural residue (i.e. straw, corn stover), forest residue (branches and tops of the trees), whole tree, and energy crops can be used to produce a range of fuels and chemicals. In Denmark, biomass currently accounts for approximately 70% of renewable-energy consumption, mostly in the form of straw, wood and renewable wastes. Consumption of biomass for energy production in Denmark more than quadrupled between 1980 and 2005 [1, 2]. The consumption of biomass (straw, woodchips) for electricity and district heating has increased significantly.

Biomass conversion can be divided into two main pathways: thermochemical conversion and biochemical conversion [3]. Biomass can also be refined through essentially mechanical treatment such as extraction (e.g. oil from seeds) or pelletizing. The thermochemical pathway can be further subdivided into combustion, gasification and pyrolysis [4]. Biomass combustion is widely applied to generate heat and electricity on a wide range of scales. Gasification converts the biomass into a gas that can subsequently be used to generate heat and electricity or be converted into fuels or other chemicals [4-6]. Pyrolysis converts the biomass into a mixture of char, liquid and gas, and is usually considered as a pre-treatment option for long-distance transport. The biochemical pathway can be divided into two main paths: digestion and fermentation into methane and ethanol, respectively [3]. Other biochemical pathways are also possible, such as anaerobic production of acetone and butanol together with ethanol [7], but less attention is devoted to them today. The conversion of biomass to polygeneration output via gasification and combustion technologies is a renewable technology that could substitute fossil fuels [8-12].

The energy related CO_2 emissions are responsible for the majority of Denmark's total emissions of greenhouse gases, approx. 78 percent in 2009 [1]. Therefore, the energy baseline scenario has large impact on the expectations for future emission levels and possible deficits in relation to international obligations.GHG emissions from agricultural sectorare predominantly relevant to facilitate a more sustainable development, and to achieve the stabilized GHG emissions and global mean temperature targets of the 1997 Kyoto Protocol and the 2009 Copenhagen Accord. In this context, Denmark is committed to a 21% reduction in GHG emissions from 1990 to 2012 [13], and has in addition agreed a national ambition of a society independent of fossil fuels by 2050.The annual GHG emissions from the primary agricultural sector in Denmark in the form of nitrous oxide (N_2O) and methane (CH_4) are currently about 10 Tg(1 Tg=10^9kg)carbon dioxide equivalents (CO_2-eq.) compared to total emissions of 66 Tg CO_2-eq. for Denmark in 2010 [14]. Furthermore, around 5 Tg CO_2-eqshould be added CO_2 emissions from direct and indirect fossil energy use [15], and a net mining of the soil carbon pools (DC) amounting to less than 1 Tg CO_2-eq. [16]. Other GHG contributions from agriculture are negligible. Methane and nitrous oxide emission from agriculture amounted in approx. 15 percent, emissions from waste (landfill) and discharged water amounted to approx. 2 percent and energy-related emissions amounted for approx. 3 percent [17].

There are few studies which have done comparative analyses of different biomass feedstock conversion pathways for biofuels and hydrogen [12, 18-20] but none of these studies investigate different biomass conversion technologies for producing power, heat, methanol, and methane from straw and wood chips. The objective of this paper is to quantify environmental impact in terms of emissions and NERs for different quad-generation production pathways. Two different technologies for producing four products are analyzed: circulating fluidized bed (CFB) and gas technology institute

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(GTI). These technologies are described in subsequent sections.

II. QUAD-GENERATION SYSTEMS

A. Quad-generation pathways

Biomass fueled combine heat and power (CHP) plants have now for many years been a common part of the Danish electricity and district heating supply. The development of energy-efficient production technologies has made cogeneration and tri-generation possible, and now, the development trend is moving towards quad-generation and poly-generation. The net energy ratio analysis has done for quad-generation. Table 1 gives the description of quad-generation plant size description and technologies.Sixteen different pathways have been considered in this study. Fig. 1 shows the different conversion pathways.

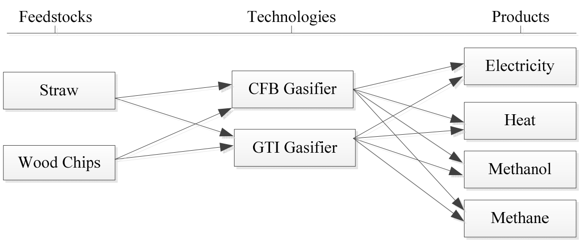


Fig.1 Biomass conversion pathways for quad-generation

B. Methodology

The quad-generation plant is produced syngas via gasification which is then used for generating power, heat, liquid fuel (methanol) and gaseous fuel (methane). Different products production pathways are analyzed as a combination of several unit operations. Materials, equipments, and fuel-embodied energy and emissions factors are determined for each of the unit operations involved in a conversion pathway over its life cycle.

Since power, heating, liquid and gaseous fuels are measured in different units (e.g. MJ, kW and m^3); the functional unit is defined as the use of 1MJ of syngas in either one of these applications. It means the quantity of a service (power, heat, methanol and methane) that is delivered by '1 MJ of syngas'. These values are the basis for the calculation of the net environmental benefit, which is used to compare the environmental advantages resulting from the substitution of different reference systems by syngas systems. It is calculated therefore as the difference between the impacts generated by syngas and reference systems. This study evaluates the NERs for all quad-generation pathways, a crucial ratio for the assessment of renewable systems. The NERs for the pathways are calculated using Eq. (1) [12].

$$NER = \frac{\sum E_{out}}{\sum E_{in}} \quad (1)$$

where, $\sum E_{in}$ = life cycle non-renewable primary energy input corresponding to the functional unit (FU) of a pathway, and $\sum E_{out}$ = energy available from the FU equivalent MJ syngas produced from the pathway. It should be noted that this study is based on the lower heating value (LHV) for fuels. Two environmental stressors i.e. net GHG emissions and acid rain precursors (ARP) are considered for emission analysis. These two environmental stressors for a particular conversion pathway are calculated using Eq. (2) [12].

$$\text{Net emission} = \sum e_{out} \quad (2)$$

where, $\sum e_{out}$ = life cycle emissions corresponding to the FU of a pathway within the defined system boundary (Fig. 2). GHG stressors are reflected to be mainly carbon dioxide (CO_2), carbon monoxide (CO), methane (CH_4), and nitrous oxide (N_2O). GHGs contribute to global warming. The global warming potential (CO_2eq) for these gases are assumed to be 1, 3, 21, and 310 respectively.

Energy consumption and emission are estimated for all the unit processes. All the key activities from farming to quad-production have been considered apart from the irrigation and electricity distribution to the grid and final consumer. A consolidated system boundary for the current LCA study is showed in Fig. 2.

To compensate for variations in electricity demand during the day and the year, the power generated at the farm is assumed to be supplied to the Danish national grid and from there retrieved by the households

Table 1. Plant size for Quad generation pathways

Technology	Feedstock	Optimum size	Comments/ Sources
CFB	Straw	1000 dtpb	These key features have been derived from an earlier study by Ruhul and Kumar [12]. The size of the each gasifier unit is assumed to be 1000 dry tonnes per day (dtpd).
	Wood chips	1000 dtpb	
CFB	Straw	1000 dtpb	The size of the plant is derived from Sarkar and Kumar [10]. The capacity of each gasifier unit is assumed to be 1000 dtpd.
	Wood chips	1000 dtpb	

III. ASSUMPTIONS OF UNIT PROCESSES

The unit processes that have been considered for CFB and GTI technologies are: Biomass production/ Supply (mainly includes seeding, production and distribution of fertilizer, herbicide and pesticide production and distribution, harvesting, manufacturing and decommissioning of all the equipments used in every stage, raking, baling, bale moving and wrapping), biomass transportation (mainly includes loading and unloading, transportation by truck), plant construction, maintenance and decommissioning, plant operation, (mainly includes shredding, plant utilities, ash disposal and regular operation) and quad-productions (mainly includes power, heat, methanol and methane production, methane transportation).

A. *Biomass production/ Supply*

Denmark is in a very superior position regarding utilization of straw, partly because energy politics since the beginning of the eighties have put a strong effort in implementing biomass in the energy supply, and partly because straw is a very essential biomass resource in Denmark [21]. For the period from 2004 to 2008 the total straw production in Denmark was 5.5 mill tons/year (82.5 PJ at 15% water) where 1.4 mill tons was used for combustion. This gives a surplus of 2.2 mill tons straw per year or 40% of the total production [1]. The straw-to-grain ratio is assumed to be 1.1:1 on the basis of its mass fraction [22]. Accordingly, a portion of the impact from common operations for straw and grain (from cultivation to harvesting) is allocated to straw. Wood chips are also only harvested in softwood stands, but by producing wood chips from hardwood, such as beech, the yield of wood chips can be greatly increased when using nurse trees. By planting hybrid larch also, the yield of wood chips could be tripled in proportion to a pure beech stand. It is justified to believe the machinery selection with agricultural practices to be more common.

B. *Biomass transportation*

As an operation in the collection process, straw is transported as bales from the field to the road side. Then these bales are transported to the power plant. In a complete life cycle analysis of freight transportation, life cycle phases of vehicles, infrastructure and fuels have to be included [23-25]. However, since the plant location is not exactly determined in the study, the infrastructure for transportation which includes the construction and maintenance of roads is assumed as already existing and no significant road construction required. It has been assumed that an average transport distance from the forest road to the plant of 20 km (own calculation), and that transport takes place with 25 t lorry.

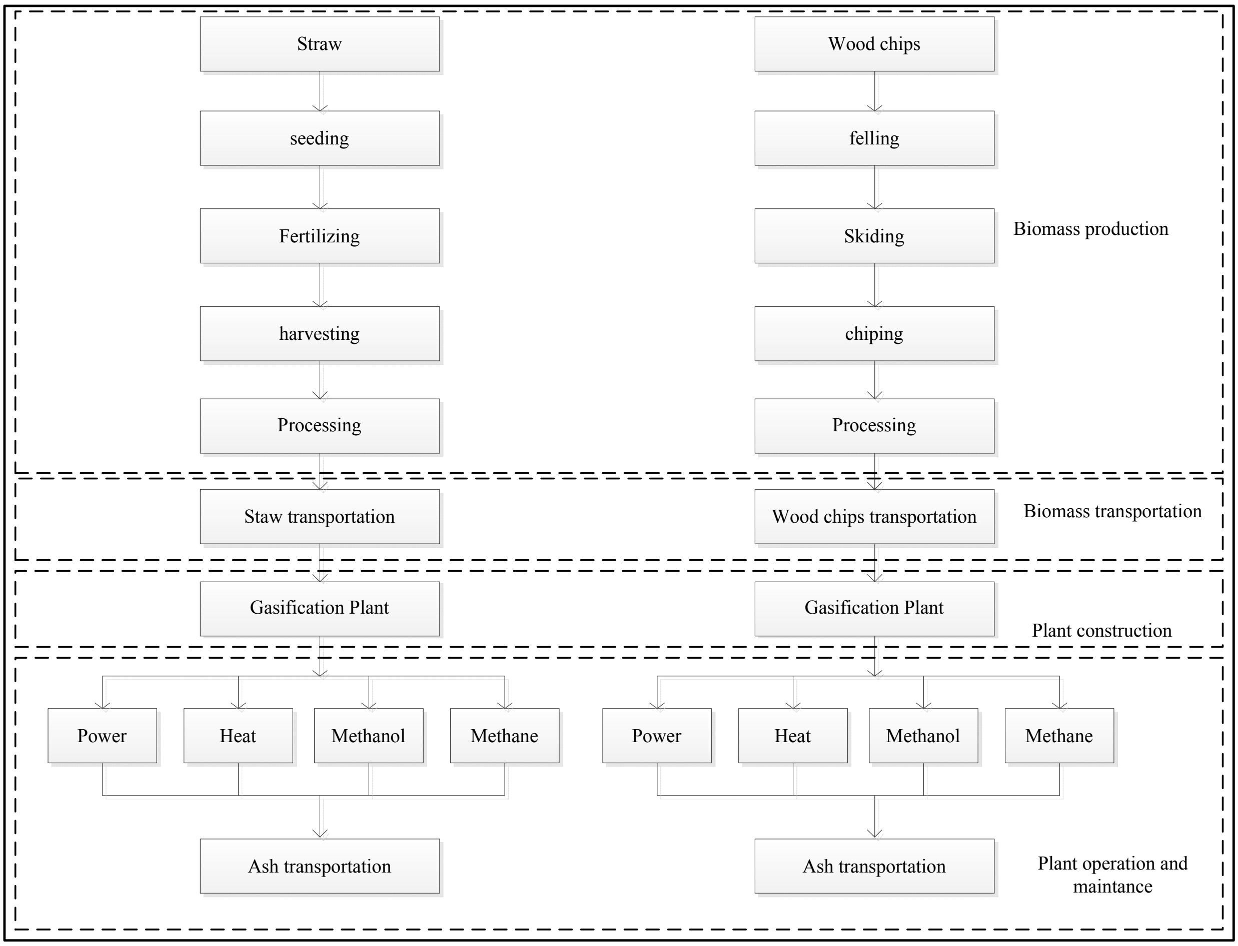


Fig 2: System boundary for quad-generation pathways

C. *Plant construction, decommissioning & disposal*

The construction material required for the different plants is estimated using data given in earlier studies [12, 26]. Scale factors are assumed to be 0.76, 0.68, 0.78 and 0.70, respectively, for BCL, GTI plants and are based on detailed analyses reported in earlier studies [10, 11]. Scale factor is defined by the following equation [27].

$$\frac{C_i}{C_o} = \left(\frac{S_i}{S_o}\right)^n \quad (3)$$

Where C_i, C_o = cost at size i and at reference (o) units, respectively. S_i, S_o = size or rating of the corresponding units, and n is the scale factor. Note that, material-embodied energy and emissions are considered over their life cycle.

D. Plant operation and maintenance

The major environment benefit of biomass energy is that theoretically it's a carbon neutral energy source once the full life cycle is considered. In simple, the CO_2 emitted during the conversion of biomass energy is considered to be the atmospheric CO_2 absorbed by the plants during the growth phase. However, this balance exists between the biomass growth and conversion emissions only.

1. Circulating fluidized bed (CFB) gasifier

The circulating fluidized bed (CFB) gasification technology is used [28] for this study. Several alternative gasification technologies exist (energy efficiencies, suitability for SNG, and other process details are discussed in [29, 30]. The CFB gasification process consists of separate gasification and combustion chambers. In the gasification chamber, hot steam and the bed material olivine are used as energy carriers to gasify wood under the absence of oxygen. The resulting producer gas consists of hydrogen, carbon monoxide, carbon dioxide, and methane as well as other hydrocarbons, tars, and ash. In the combustion chamber the energy required to maintain this endothermic process is transferred to steam and olivine through the combustion of wood and incompletely gasified wood fractions (coke and tars). During gasification, tars as well as other substances are formed from traces of nitrogen, sulphur, chlorine, and metals contained in the wood and transferred into the product gas, from which it needs to be cleaned. This is done in several steps including a baghouse filter to remove particles as well as a washing step with rape methyl ester (RME) as organic solvent to remove water and tars.

2. Gas Technology Institute (GTI) gasifier

In the case of GTI pathways, the electricity produced by the plant is enough to support the feedstock pretreatment processes and other plant operations [31]. Once again, credits from selling extra electricity to the grid are not considered. In addition, natural gas need not be purchased for these pathways. So, for GTI pathways ash disposal is the only plant operation that needs to be accounted for.

E. Quad production

This unit process is relevant to both CFB and GTI pathways. It includes power, heat, methanol and methane production. It is assumed that the quad-generation plant has access to the national natural gas grid. In this context, a process that converts biomass into methane does not require any transportation. It is assumed that, methanol is transported for 200 km. Methanol has low density that only 300 kg methanol can be carried using a conventional 36 tonne payload truck [32].

IV. Inventory Assessment for Life Cycle Calculation

A. Biomass properties and plant characteristics

The yield and physical properties of biomass are very critical to performing NER analysis for biomass-based systems. These have a significant impact on various upstream and downstream operations of biomass conversion such as transportation, feedstock pretreatment, plant mass and energy balance, plant maintenance, etc. The biomass inventory data and general plant assumptions are given in Table 2.

Table 2: Biomass properties and general assumptions

Properties	Units	Straw	Wood chips	Comments/ References
Moisture content	%	7.5-12	45	These are the moisture contents of as received feedstocks. It is assumed that moisture contents wouldn't change transportation of feedstocks after preliminary processing [33, 34]
Bulk density	kg/m^3	130	300	-
LHV	MJ/dry kg	15	10.5	[34, 35]
Ash	%	4	-	[36]
Plant operating factor	-	-	-	These are conventional operating factors being used for biomass based plants[37]
Year 1	0.7		0.7	-
Year 2	0.8		0.8	-
Year 3	0.85		0.85	-

B. Fuel and fertilizer requirement

Almost all the unit processes used fossil fuel as the primary energy input. Methanol is required to methane and methanol production. Almost 68% of all the electricity generated in Denmark comes from fossil fuel-fired power plants [1, 2]. Therefore, there are high emissions related to grid electricity. These emissions are estimated on life cycle basis. The efficiency with which natural gas is converted to electricity is assumed to be 45%. Table 3 also shows the life cycle energy and emissions factors for different fertilizers and pesticides. The transportation inventory data include the production, use and disposal of trucks.

C. Inventory data for plant construction, decommissioning, and disposal

There aren't many studies with primary energy and emissions related to decommissioning of a power plant. The steel, concrete and aluminum required to construct a GTI plant (for processing straw and woodchips), the material required is

Table 3: Energy input/output ratio and emission factors for electricity, different fuels and chemicals [12, 26, 3841]

Items	Diesel	Natural gas	Methanol	Electricity (unit/MWh)	Fertilizer (Unit/kg)			Pesticide (unit/kg)
					N	*P*	*K*	
LHV (MJ/kg)	46.03	49.1	22.7	-	-	-	-	-
Density (kg/m^3)	832	0.78	792	-	32	96.01	-	-
kg CO_{2eq}/GJ	94.2	56.6	16	820	3.27	1.34	0.64	24.5
kg SO_{2eq}/GJ	0.37	0.13	2.00e-03	0.57	0.38	0.4	0.4	2.96
kg (NO_x+VOC)/GJ	0.59	0.22	1.00e-03	0.585	0.4	0.41	0.41	3.01
GJ/GJ	1.22	1.11	0.04	2.86	0.05	0.01	0.004	0.12

5084, 15,720, and 42 tonnes, respectively. To construct a CFB plant construction (for all the feedstocks), the necessary amount of steel, concrete and aluminumare needed almost 5350, 16,535, and 44 tonnes, respectively [1, 6, 40]. However there are details of some limited research on this issue. According to these studies, primary energy input and relevant CO_2 eq. emissions for decommissioning are in-between 3% to 5% of energy and emissions associated with the plant construction. Therefore, the decommissioning impact is assumed to amount to 3% of the construction impact [42] for all plants.

Table 4: Methanol transport inventory data [12]

Mode	Category	Values	Comments/ Sources
Truck	Energy impact	0.85 $MJ \cdot m^{-3} km^{-1}$	Impacts include truck manufacturing, infrastructure construction, and truck operation. The authors evaluated other impacts based on the material inventory
	Emission Impact	56 $gmCO_{2eq} m^{-3} \cdot km^{-1}$	
		0.23 $gmSO_{2eq}\ m^{-3} \cdot km^{-1}$	
		0.36 kg (NO_x+VOC) $\cdot m^{-3} km^{-1}$	

D. *Inventory data for plant operation and maintenance*

The natural gas required to produce individual output from quad-generation using CFB gasifier has been found to be 0.12 m^3/m^3 syngas for both of the feedstock [28, 29]. Neither natural gas nor electricity purchases are required for GTI-gasifier-based quad-generation [30]. Methanol (10 wt.%) is needed both for methanol and methane production. Inventory data for methanol have been given above table 3. Ash is disposed 50 km away from the plant and is spread (1 tonne ash/ha) to replace nutrients [12]. The ash content in methanol and methane is less than 0.1%, hence, the impact from ash disposal is ignored in this study. The cleaned producer gas is used in a gas-powered heat, power, methanol and methane unit. Many studies have assumed a percentage of plant construction energy as the maintenance energy of the power plant, mostly between 2.5% to 5% [42]. In this study, energy and emissions of plant maintenance is assumed to be 3% of the plant construction energy and emissions in both cases.

E. *Recycling and waste disposal*

Steel, Iron and Aluminum used in all machinery, plant equipment and construction are considered to be recycled. The amount of steel used in farm machinery is considered as 98% wherever it's not possible to find the exact value [43].The energy and emissions needed to recycle these materials are considered in the analysis.

F. *Inventory data for methanol transportation*

Methanol has high density of 792 kg/m^3. This makes truck as a favorable mode of transportation along with the pipeline. It is assumed that methanol blend will be transported either using B-train truck of 60 m^3 capacity. Inventory data for methanol transportation are presented in Table 4.

V. RESULTS AND DISCUSION

A. *Life cycle energy impact*

The total energy impact and NER corresponding to the functional unit for different GTI and CFB pathways are shown in Table 5. Note that, in order to determine NER, the LHV of methanol and methane has been assumed to be 19.6 $MJ/NM^3$and 38 MJ/NM^3 respectively [45]. Fig. 3 shows the energy break down in all unit processes during the life cycle of quad- production for both straw and wood chips. In case of CFB pathways, the total energy impact for the both biomass feedstocks are comparatively higher than GTI pathways as plant operation and maintenance contributes significantly to the overall energy impact. Life cycle energy consumption corresponding to one functional unit is higher for fast CFB pathways. The main reason is the feedstock pre-treatment and energy input for CFB. So, energy from framing and harvesting is almost double. In addition to that, more transportation distance is needed to be covered. To sum up, NER for quad-production pathways is in the range of 1.3-7.2. In contrast, coal and natural gas based bio-oil production plant demonstrates NER in the range of 0.57-0.67 [26, 41].

B. *Life cycle emission impact*

Life cycle GHG emissions from different pathways are depicted in Fig.4. No greenhouse gas (GHG) emissions are generated during biomass growth. Wood transport by truck over short distances is rather efficiency and thus the use of diesel and generated air emissions only cause small impacts. Life cycle emission consumption corresponding to one functional unit is higher CFB straw pathways. The main reasons behind it are: net straw requirement for the same amount of power production is almost twice as syngas yield

Table 5: Life cycle energy performance of quad-generation pathways

Feedstocks	Technologies	Pathways	MJ/MJ Syngas	Kg CO_{2eq}/MJ syngas)
Straw	CFB	PW 1	5.8661	1.1513
		PW 2	7.2153	1.9733
		PW3	7.1243	1.9733
		PW4	6.8450	1.9733
	GTI	PW 1	3.1562	0.2158
		PW 2	3.2959	0.2158
		PW 3	3.3257	0.2158
		PW 4	3.0525	0.2158
Wood chips	CFB	PW 1	4.3710	1.8797
		PW 2	4.2212	1.8797
		PW3	4.4141	1.8797
		PW4	4.2036	1.8797
	GTI	PW 1	1.2694	0.1847
		PW 2	1.7669	0.1847
		PW 3	1.9544	0.1847
		PW 4	1.3703	0.1847

has been assumed as 50 wt% from triticale straw. It also has a similar reason for CFB wood chips pathways. Fig. 5 shows the Life cycle acid rain precursor emission for straw and wood chips in CFB and GTI technologies. Based on this LCA study GHG, ARP emission intensities for quad-generation production are in the range 0.24 to 4.41 Kg CO_2eq/NM^3 syngas and 0.03 to 0.84 Kg SO_2eq/NM^3 respectively.

C. *Sensitivity analysis*

A sensitivity analysis with following scenario is carried out in this study. Scenario 1 consider excluding the farming and harvesting inputs. Hence, the feedstocks can be regarded as waste material energy need not to be allocated to feedstocks as it was in the base case. If the plant efficiency is improved from 64 % to 69 % for gasification plant, scenario 2 develops for plant efficiency improvement. Scenario 3 suggests that, exclusion of silviculture and road construction from WF biomass reduces the impacts significantly compared to all the pathways. Effects of 10% increase or decrease in syngas yield is analyzed in scenario 4. This scenario is developed for both straw and wood chips. Scenario 5 consider higher operating factor for the plants (0.7 for year 1, 0.8 for year 2 and 0.95 from year 3 onwards). Based on the scenarios considered, LCA was performed again to analyze their impact. Findings have been summarized in Table 6.

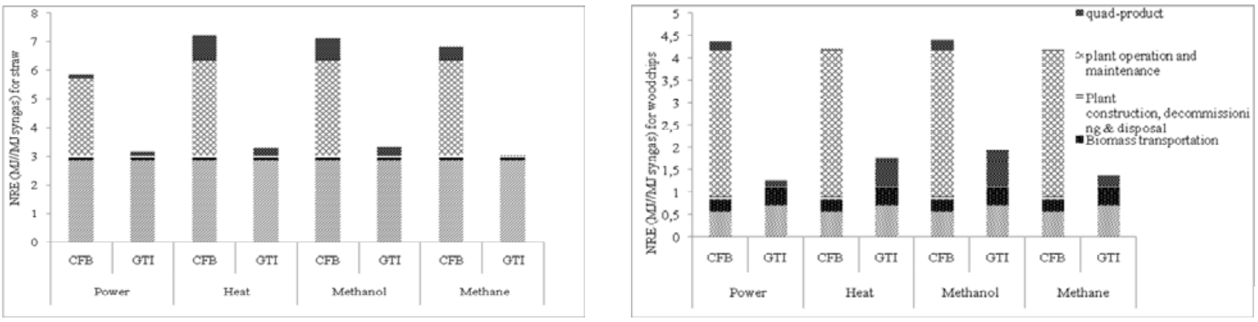
VI. CONCLUSIONS

The study has been done to determine the net energy ratio and environmental advantage of using straw and wood chips for quad (power, heat, methanol and methane) production as a continuation of Denmark's quest on increasing the renewable energy penetration in its energy sector. Two conversion pathways have been considered taking straw and wood chips as the sustainable energy option. Among the CFB pathways, straw based heat production pathway has maximum NER of 7.22. Similarly, among GTI pathways also, straw based methanol production pathway has maximum NER of 3.33. For CFB and GTI production pathways, use of woodchips for heat production, produces lowest GHG emission and use of woodchips for methanol production, produces less amount of acid rain precursor among the other options.By increasing the share of wind power in total energy system, reducing the use of fossil fuels use in energy production and replacement of those fossil fuels with domestic biomasses will represent the main means of GHG emissions saving in the future energy system.

Table 6: Key sensitivities and their results

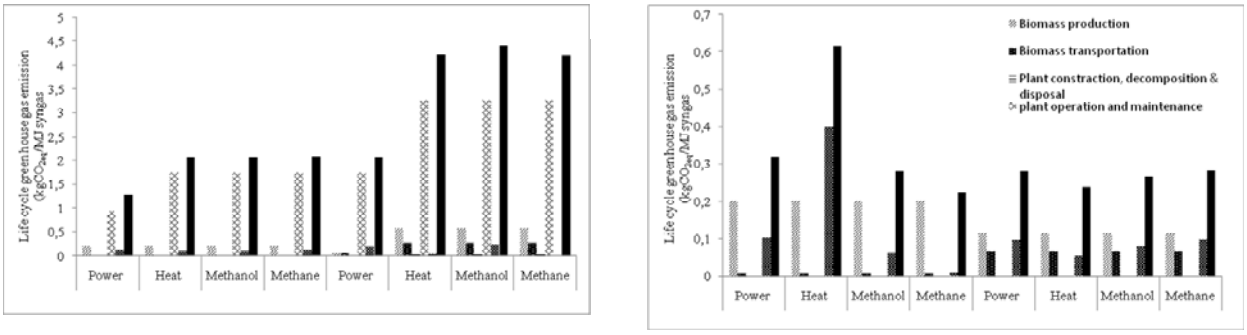
Scenario		Conversion Patways	Energy (MJ//MJ syngas)	Change fom base case	GHG (kg CO_2e/MJ syngas)	Change	ARP (kg SO_2e//MJ syngas)	Change
1	**Straw**	CFB	6.76	-26%	1.28	-25%	6.9e-01	-28%
		GTI	3.207	-30%	0.32	-32%	3.6e-02	-30%
	Wood chips	CFB	4.37	-17%	2.07	-18%	0.10	-19%
		GTI	1.26	-10%	0.28	-15%	7.4e-01	-13%
2		CFB	1.50	-14%	0.37	-19%	4.7e-01	-19%
		GTI	1.50	-14%	0.37	-19%	4.7e-01	-19%
3	**Wood chips**	CFB	4.37	-17%	2.07	-16%	0.10	-34%
		GTI	1.26	-10%	0.28	-19%	7.4e-01	-19%
4		CFB	2.43	-39%	0.79	34%	4.9e-02	-36%
		GTI	1.85	-22%	0.28	19%	3.6e-01	-12%
5	**Straw**	CFB	6.76	-26%	1.28	-36	6.9e-01	-28%
		GTI	3.207	-30%	0.32	-	3.6e-02	-30%

CFB= Circulating fluidized bed, GTI = Gas Technology Institute, pathways.



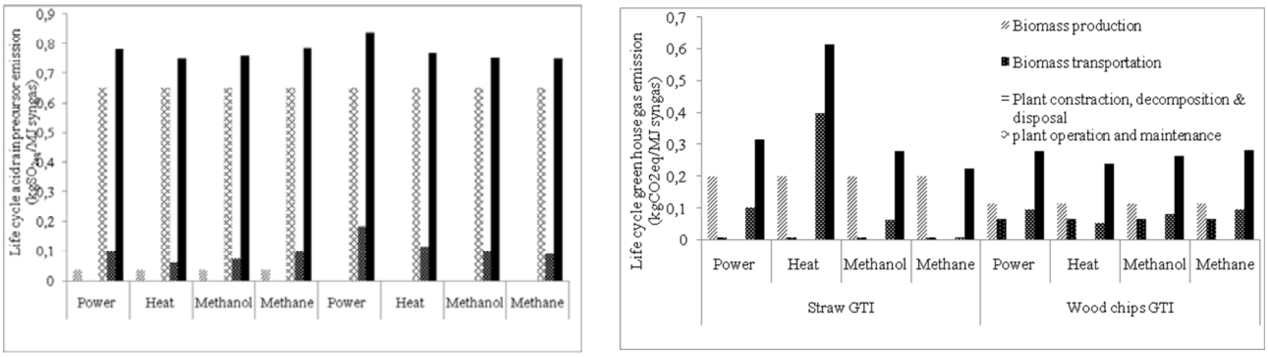
(a) (b)

Fig. 3: NER graphs for both (a) straw and (b) wood chips



(a) (b)

Fig.4 Life cycle CO_2 emission from (a)CFB and (b) GTI pathways



(a) (b)

Fig 5: Life cycle acid rain precursor emission for (a) CFB and (b) GTI pathways

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Paper 6

A performance analysis of integrated solid oxide fuel cell (SOFC) and heat recovery steam generator (HRSG) for IGFC system.

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RESEARCH ARTICLE

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A performance analysis of integrated solid oxide fuel cell and heat recovery steam generator for IGFC system

Abstract Solid oxide fuel cell (SOFC) is a promising technology for electricity generation. Sulfur-free syngas from a gas-cleaning unit serves as fuel for SOFC in integrated gasification fuel cell (IGFC) power plants. It converts the chemical energy of fuel gas directly into electric energy, thus high efficiencies can be achieved. The outputs from SOFC can be utilized by heat recovery steam generator (HRSG), which drives the steam turbine for electricity production. The SOFC stack model was developed using the process flow sheet simulator Aspen Plus, which is of the equilibrium type. Various ranges of syngas properties gathered from different literature were used for the simulation. The results indicate a trade-off efficiency and power with respect to a variety of SOFC inputs. The HRSG located after SOFC was included in the current simulation study with various operating parameters. This paper describes IGFC power plants, particularly the optimization of HRSG to improve the efficiency of the heat recovery from the SOFC exhaust gas and to maximize the power production in the steam cycle in the IGFC system. HRSG output from different pressure levels varies depending on the SOFC output. The steam turbine efficiency was calculated for measuring the total power plant output. The aim of this paper is to provide a simulation model for the optimal selection of the operative parameters of HRSG and SOFC for the IGFC system by comparing it with other models. The simulation model should be flexible enough for use in future development and capable of predicting system performance under various operating conditions.

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Keywords SOFC, HRSG, IGFC, syngas

1 Introduction

The behavior of coal contaminants toward a potentially clean, highly efficient integrated power-generating system is becoming increasingly important for both a system's performance and endurance. Integrated gasification fuel cell (IGFC) is an integrated power-generation system that combines integrated gasification combine cycle (IGCC) and high-temperature fuel cells. The fuel cell system is more expensive than a combustion turbine, but is counterbalanced by the decrease in the unit cost of upstream equipment due to higher IGFC system efficiency [1]. A wide variety of coals be used, allowing for the effective use of coal. Low-grade coals with high moisture content and low calorific values, such as brown and sub-bituminous coals, are difficult to use in conventional pulverized coal-fired power generation, but they can be used as fuel for IGCC or IGFC power generation through a relatively easy gasification process [2]. IGFC systems are promising for efficient and clean power generation from domestic resources, but most IGFC system analyses performed to date have used non-dimensional solid oxide fuel cell (SOFC) models that do not resolve many intrinsic constraints of SOFC operation. A simplified cell-level SOFC model will provide more insights on the SOFC operation at a reasonable computation expense. A finite volume model is a possible choice [3]. A hybrid system of SOFC with gas turbine has been extensively studied in the field of energy conservation. A literature survey indicates that past research and development of SOFCs for large power systems has made significant advances since the early 1990s [4]. Fuel cell system control and design have received increasing attention throughout the years, considering the energetic and economic aspects and using sensitivity analyses [5]. George [6] described a field unit demonstration program including the Southern California Edison 220 kW pressurized SOFC/gas turbine (PSOFC/GT) power system, along with planned demonstrations of commercial prototype power systems from Siemens Westinghouse Power. In terms of heat exchangers and heat recovery steam generators (HRSGs) characterized by a tube-in-tube counter flow arrangement, simulation was conducted using the thermal efficiency-NTU approach [7]. The energy and exergy were analyzed not only for the entire plant but also for each component to evaluate the distribution of irreversibility and thermodynamic inefficiencies.

HRSG is a key component of any IGFC design, and is used to convert heat energy in the SOFC exhaust gas into steam, which is then sent to a steam turbine to augment the power from the SOFC output. It also presents a way to reduce pollutant emissions. The main heat source of HRSG, which is the exhaust from the SOFC, changes significantly because of the change of load and ambient temperature. The inlet temperature and mass flow rate of the HRSG gas often vary greatly. High-pressure steam is delivered to the steam turbine in a sliding pressure mode. Heat and mass transfer of water and steam is accompanied by a multi-system, multi-direction, and multi-form [8, 9]. The performance of HRSG strongly affects the overall performance of the power plant. The optimization of the HRSG is only the first step in the optimum design of the entire plant.

In this paper, a simulation model of an integrated SOFC and HRSG for the IGFC system was created. Considering the contribution of the different components of the cycle, an algorithm was developed using Aspen Plus to simulate the performance of SOFC for the IGFC cycle. The simulation investigated the effects of various performance parameters, such as SOFC fuel, air inlet temperature, and flow rate. Finally, the output gas from the SOFC was utilized for the HRSG simulation, and temperature profile for HRSG was represented graphically.

2 Model description

The gasifier modeled in this application is based on the concept of coal gasification to produce high-methane-content syngas at a relatively low operating temperature, which benefits both gasifier efficiency and SOFC performance. The integrated SOFC-HRSG layout is schematically illustrated in Fig. 1. The whole power plant system is described as follows.

1) Coal is gasified in the gasifier.

2) Oxygen is pumped from a cryogenic air separation unit into the gasifier and then into the SOFC after being heated in a heat exchanger.

3) Particulate is removed from the raw syngas exiting the gasifier using a cyclone collector and a candle filter system.

4) Sulfur-free syngas from the gas-cleaning unit serves as fuel for the SOFC. At the stack, fuel is mixed with the anode recirculation stream to support the steam reforming reaction in the pre-reformer and in the anode compartment

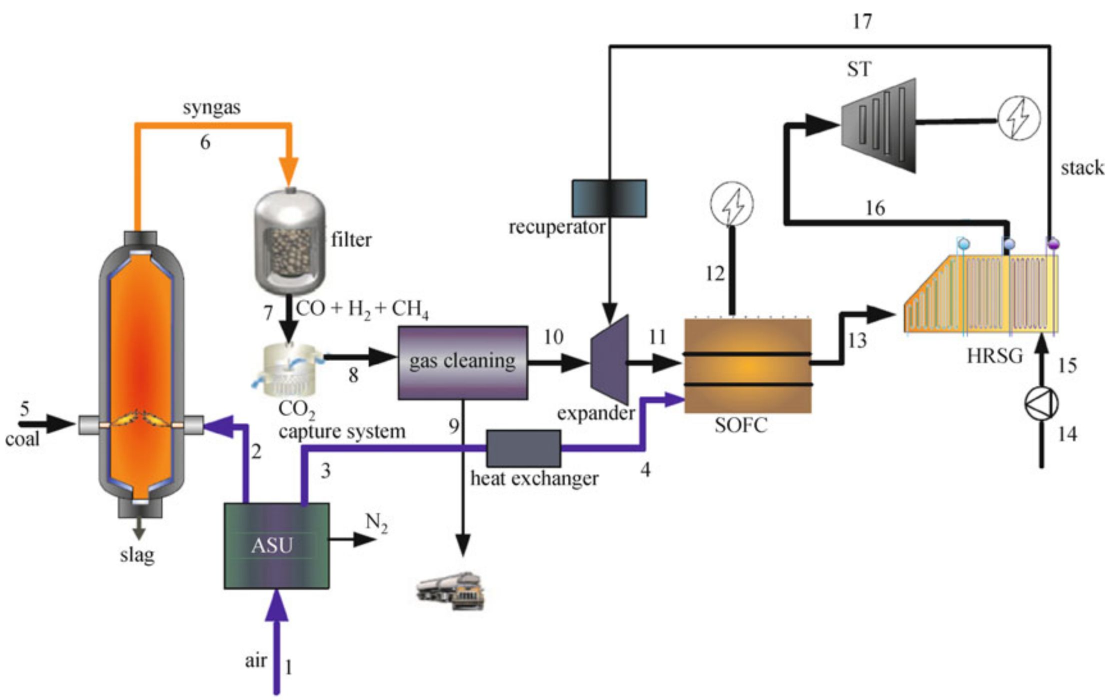

Fig. 1 Simplified flow diagram of the integrated SOFC-HRSG model in the IGFC plant

of the fuel cell. The non-reacted fuel is involved in the internal reforming reaction within the anode compartment of the SOFC stack.

5) The electrochemical reactions occurring in the fuel cell produce DC electrical current and release thermal energy. The DC electrical current is converted into AC by the inverter, while the thermal energy is used by the internal reforming reaction to heat up the fuel cell stack.

6) The SOFC exhaust stream flows to the HRSG. The gas mixture side of the HRSG passes through the heat exchanger sections — high-pressure (HP) superheater (SU), reheater (RH), HP evaporator (EV), HP economizer (EC), intermediate-pressure (IP) SU, IP EV, IP EC, low-pressure (LP) SU, LP EV, and LP EC — and is exhausted at the stack.

7) The superheated steam produced by the HP SU is supplied to the HP stage of the steam turbine. After expansion, the cold reheated at an intermediate pressure returns to the HRSG and, through a reheater, is superheated and returned to the IP/LP steam turbine stage. The IP SU and the LP SU superheat the steam to the double-admission IP/LP steam turbine, which during expansion produces mechanical power that is in turn converted into electric power in a generator.

In Fig. 2, a simple model that is part of this simulation study is shown. Two different types of syngas properties — Pulverized Dry Coal (Illinois #6 coal) and Kideco (Dry), which are taken from the simulation previously made in the energy processes laboratory of Ajou University — were used in the SOFC simulation. The simulation is named “simulation A” for Illinois #6 coals and “simulation B” for Kideco (Dry). These syngas properties are used for the SOFC simulation in the same Aspen Plus flow sheet, and output properties of different parameters are utilized for HRSG-ST simulation. In the developed model, both fuel cell and steam turbine can produce electricity, which can be utilized by the grid connection.

3 Thermodynamic efficiency

For the SOFC, the thermal efficiency of any energy-conversion device can be defined as the ratio of useful work done W_{out} and the potential of the inlet stream to do work Q_{in}, that is, $\varepsilon = W_{out}/Q_{in}$. For a fuel-cell system, the useful work is electric power W_e, which is the product of the electric current density i and operating voltage E_{cell} integrated over the active area, $W_e = \int iE_{cell}\,dA$. The potential to do work can be represented in terms of the heat release associated with full oxidation of the inlet fuel stream, $Q_{in} = m_{f,in}\Delta h_{f,in}$. Here, the inlet fuel mass flow rate is $m_{f,in}$, while $\Delta h_{f,in}$ is the specific enthalpy associated with completely oxidizing the fuel stream. With these definitions, the net fuel-cell efficiency can be defined as

$$\varepsilon = \frac{W_e}{Q_{in}} = \frac{\int iE_{cell}dA}{m_{f,in}\Delta h_{f,in}}. \tag{1}$$

The efficiency of a fuel-cell system can be written as the product of three contributing efficiencies [10]: reversible efficiency ε_R, voltage or part-load efficiency ε_V, and fuel utilization ε_U,

$$\varepsilon = \varepsilon_R \varepsilon_V \varepsilon_U. \tag{2}$$

The ideal efficiency, or the reversible efficiency, ε_R is written as

$$\varepsilon_R = \frac{\Delta G}{\Delta H} = 1 - T\frac{\Delta S}{\Delta H}, \tag{3}$$

where ΔG, ΔH, and ΔS are the changes in molar free energy, enthalpy, and entropy, respectively, associated with full oxidation of the fuel. Any over-potential losses within the fuel cell reduce the cell potential when it is operated under load. Thus, the net efficiency depends on the operating cell potential E_{cell}. A part-load efficiency or the voltage efficiency is defined as

$$\varepsilon_V = \frac{E_{cell}}{E_{rev}}. \tag{4}$$

This approach is improved by incorporating activation–polarization losses using a two-linear-segment polarization curve. Fuel utilization significantly affects efficiency. Take an SOFC system where fuel is electrochemically oxidized along the length of an anode channel. As the fuel is consumed, the anode fuel stream is also diluted by reaction products (i.e., H_2O and CO_2). As the fuel concentration decreases along the length of the anode channel, the reversible potential E_{rev} decreases.

As long as the reversible potential exceeds the cell operating potential (i.e., $E_{rev} > E_{cell}$), the cell can produce electric current. However, once E_{rev} equals E_{cell}, no more fuel can be consumed and no more current can be

Fig. 2 Simple model for this simulation study

produced. Unused fuels in the exhaust reduce the fuel-cell efficiency. Fuel utilization ε_U can be written as

$$\varepsilon_U = 1 - \frac{m_{f,out}\ \Delta h_{f,out}}{m_{f,in}\ \Delta h_{f,in}}, \tag{5}$$

where, the "in" and "out" refer to the inlet and outlet of the fuel cell, respectively. The "Δh" refers to the specific enthalpy associated with complete oxidation of any available fuels, and "m" refers to the mass of every available fuel. This definition accounts for the energy content of any remaining fuels (or fuel by-products) that leave the fuel-cell exhaust. For example, although all the parent fuel (e.g., a hydrocarbon) is consumed in that it is no longer present in the anode exhaust, there may still be considerable energy available in the form of other hydrocarbons or CO and H_2. The reversible efficiency (ε_R) can be determined thermodynamically by Eq. (3), but it cannot be achieved in practice because of low fuel utilization at high operating potential. The efficiency reaches a maximum at an operating potential of around 0.8 V.

The steam turbine is a mechanical device that converts thermal energy in pressurized steam into useful mechanical work. It has higher thermodynamic efficiency and lower power-to-weight ratio, making it ideal for very large power configurations used in power stations.

The overall thermal efficiency of a steam turbine plant can be represented by the ratio of the net mechanical energy available to the energy within the fuel supplied, as indicated in the following expressions. Isentropic efficiency η by definition is given by

$$\eta = \frac{h_{HP} - h_{LP}}{h_{HP} - h_{LPisen}}, \tag{6}$$

where

- h_{HP} is the specific enthalpy of the steam at the turbine inlet,
- h_{LP} is the specific enthalpy of the steam at the turbine exhaust, and
- h_{LPisen} is the specific enthalpy of the steam at the turbine exhaust pressure in water.

The ratio is defined as

$$m = \frac{\eta_{FL}}{1 - \eta_{FL}}, \tag{7}$$

where η_{FL} is the turbine isentropic efficiency at full load.

The isentropic efficiency η at load P can be estimated by

$$\eta = \frac{mP}{P_R + mP}, \tag{8}$$

where P_R is the rated turbine power.

The specific enthalpy at the turbine exhaust conditions is then expressed as

$$h_{LP} = h_{HP} - \eta(h_{HP} - h_{LPisen}). \tag{9}$$

The steam consumption at operating load P is given by

$$m_s = \frac{P}{h_{HP} - h_{FL}}. \tag{10}$$

4 Aspen Plus simulation

Aspen Plus simulation software was used to develop the thermodynamic models, which simulates the behavior of the hybrid fuel cell system configuration. For this model, it is necessary to consider the following assumptions: one-dimensional flow; steady state; no gas leakage; negligible heat losses to the environment; and negligible kinetic and gravitational terms in the energy balances.

4.1 SOFC simulation model

The stream "SYNGAS" is fed to the "COMPR1" block, simulating the fuel compressor. The discharge pressure is calculated by assuming a pressure ratio of $P_{fuel}/P_{SOFC} = 3$ [11]. The syngas stream composition and thermodynamic condition are inputted; the mole flow rate is set by a design specification and depends on the specified stack power. The pressurized fuel is brought up to the block "FUELHEAT" in Fig. 3 and its exit stream enters the "EJECTOR" block, where it is mixed with the recycled depleted fuel (stream 27). The pressure of the mixed stream (stream 4) is decreased to slightly above atmospheric pressure (P_{SOFC}) and is directed to the "COOLER" block. The two blocks — COOLER and "PREFORM" — simulate the operation of the pre-reformers. The purpose of the COOLER is to set the pre-reforming temperature. It is calculated through a design specification, which changes the temperature of the COOLER until the net heat duty of the PREFORM equals zero (adiabatic). As a result, the gas is cooled, simulating the endothermicity of the steam reforming process. The following chemical reactions are specified in the PREFORM block.

Steam reforming:

$$CH_4 + H_2O = 3H_2 + CO \tag{11}$$

Water–gas shift:

$$CO + H_2O = CO_2 + H_2 \tag{12}$$

It is assumed that the reactions reach thermodynamic equilibrium at the pre-reforming temperature. The pre-reformed fuel (stream 6) is fed to the "B5" block, where the remaining CH_4 is reformed. CO is shifted and H_2 is oxidized. In an SOFC, the following reactions occur.

Cathode half reaction:

$$0.5O_2 + 2e^- \rightarrow O^{2-} \tag{13}$$

Anode half reaction:

$$H_2 + O_2 \rightarrow H_2O + 2e^- \tag{14}$$

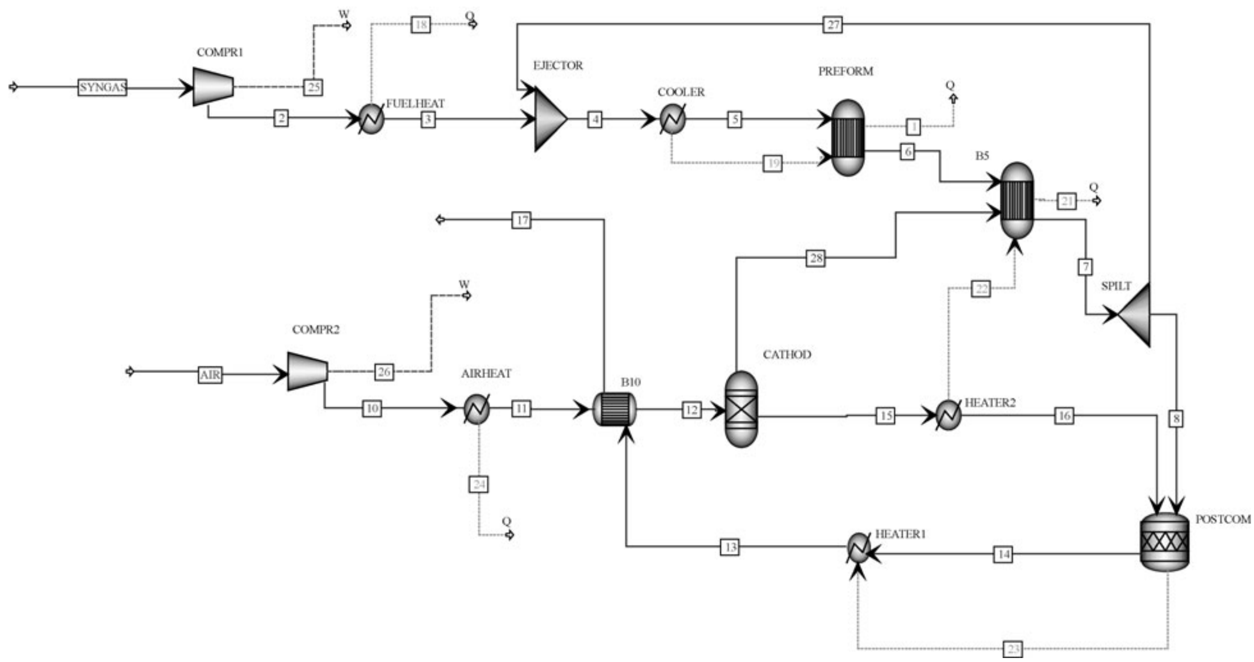

Fig. 3 Aspen Plus simulation model for SOFC

Overall reaction:

$$H_2 + 0.5O_2 \rightarrow H_2O \tag{15}$$

The oxygen ion O^{2-} is the charge carrier in an SOFC. It is transported through the electrolyte to the anode side, where it reacts with H_2 to produce electrons e^-. The transfer of ions cannot be modeled in Aspen Plus; therefore, the overall reaction — instead of the cell half reactions — was used in the simulation. Although it is possible to oxidize CH_4 and CO directly in an SOFC at its high operating temperature, it is common to assume that the CH_4 is reformed and the CO is shifted to H_2; thus, only H_2 participates in the electrochemical reaction. Reactions (11), (12), and (15) are specified in the B5 block (anode), and it is assumed that they reach thermodynamic equilibrium at the block temperature. The oxidant (stream "AIR") is fed to the "COMPR2" block, the air compressor. Its discharge pressure is set slightly above atmospheric pressure (P_{SOFC}). The air stream composition and thermodynamic condition are inputted. The molar flow rate is determined using a design specification that varies the airflow until the air utilization factor $U_a = 18\%$ [12]. The compressed air is brought up to the block "AIRHEAT" and its exit stream enters "B10". The compressed air (stream 12) enters the "CATHOD" block, whose function is to separate the O_2 required for the electrochemical reaction.

The heat needed to do this is supplied by the electrochemical reaction; this process is simulated by taking a heat stream (22) from "HEATER2" to B5 (anode). The temperature of the HEATER2 block is determined. The depleted fuel (stream 7) enters the block "SPLIT", whose function is to split the stream into a recycle (stream 8) and a stream directed to the combustion plenum. The split fraction of the block, which is defined as the molar ratio of steam to combustible carbon with standard value of 2.5, is set using a design specification. Excess steam, as well as increasing the concentration of H_2 and CO_2, inhibits the formation of carbon. Carbon deposition not only represents a loss in the system, but results in the deactivation of catalysts and decreases the activity of the anode by clogging the active sites. The depleted fuel and oxidant are fed to "POSTCOM", where complete combustion of the remaining fuel occurs. The following combustion reactions, assumed to reach completion, are specified as follows.

H_2 combustion:

$$H_2 + 0.5O_2 \rightarrow H_2O \tag{16}$$

CO combustion:

$$CO + 0.5O_2 \rightarrow CO_2 \tag{17}$$

CH_4 combustion:

$$CH_4 + O_2 = 2H_2O + CO_2 \tag{18}$$

The heat generated by the reactions is calculated and is put into the heat stream 23, which is fed to the block "HEATER1", whose function is to calculate and set the combustion products temperature. Finally, the high-temperature combustion products (stream 13) exchange heat with and serve to preheat the incoming air in the heat exchanger "B10" block.

4.2 Simulation model for HRSG in Aspen Plus

Simulation is more applicable in HRSG, as it has several operating conditions like multiple levels of steam pressure, temperature, and mass flows. However, simulation may also be applied to other waste heat recovery applications involving clean gas streams. This paper does not compute surface areas, tube sizes, or geometry in the simulation. While planning or developing IGFC projects, various SOFC, steam parameters, and operating conditions should be evaluated to see which is best for the plant and what could happen to the entire system due to the HRSG behaviors at certain points [13]. Simulation saves much time, as some parameters and operating conditions can be easily confirmed and others eliminated; the few possible options for gas and steam conditions are then further studied. Almost all performance information (gas-steam temperature profiles, steam generation, amount of supplementary fuel, gas analysis before and after the burner, and fuel inputs with SOFC exhaust) are available at this stage; hence, the specifications for the HRSG can be written more clearly.

The steam cycle used for these cases is based on a design by the process division DOE. The cycle is a three-pressure-level reheat process. Major components include an HRSG, steam turbines (high, intermediate, and low pressure), a condenser, a recycle water heater, and a de-aerator. The differences are related to the heat integration, which is possible with the gasifier island sections, including raw fuel gas being cooled at 815°C. This reduces the amount of high-pressure steam generated in this exchanger. The reduction occurs due to the two additional high-quality heat sources in the heat exchanger prior to reaching the acid plant and in the heat exchanger used to cool the recycled quench gas.

The condensate from the steam condenser that uses low-quality heat is reheated at 152°C. A bleed of low-quality steam is used to heat the condensate further to 136°C, increasing the makeup water requirements for the steam cycle.

Steam generation occurs at the three pressure levels of 95700, 1952, and 392 kPa in the HRSG. The cycle includes a parallel superheating/reheating section that raises the temperature to 538°C for both the high-pressure steam and the combined intermediate pressure steam and high-pressure turbine exhaust steam. Compressors, fans, and turbines can all be simulated in Aspen Plus by a block called COMPR. The COMPR models polytropic and positive displacement compressors, isentropic compressors, and turbines, as well as fans. It calculates the power required (or produced) given the pressure ratio, isentropic, polytropic, and mechanical efficiencies and, for positive displacement compressors, the clearance volume. The accuracy of the results depends on the efficiencies specified. The COMPR block in the isentropic mode calculates the net work output from the change in enthalpy for isentropic expansion.

In the models used here, the steam turbine stages in the HP and IP sections and the first two stages of the LP section are modeled using COMPR blocks. As an example, the schematic layout for the IP turbine and the corresponding Aspen Plus flow sheet are given in Fig. 4.

For each section of the turbine, steam inlet and exit pressures and temperatures are available from the literature data. Thus, the polytropic efficiency of the entire section is first calculated iteratively from the known steam inlet and exit conditions assuming constant polytropic efficiency throughout the section, as proposed by Erbes and Eustis [14]. Using the constant polytropic efficiency and reheat factors, the expansion line for the section and the isentropic

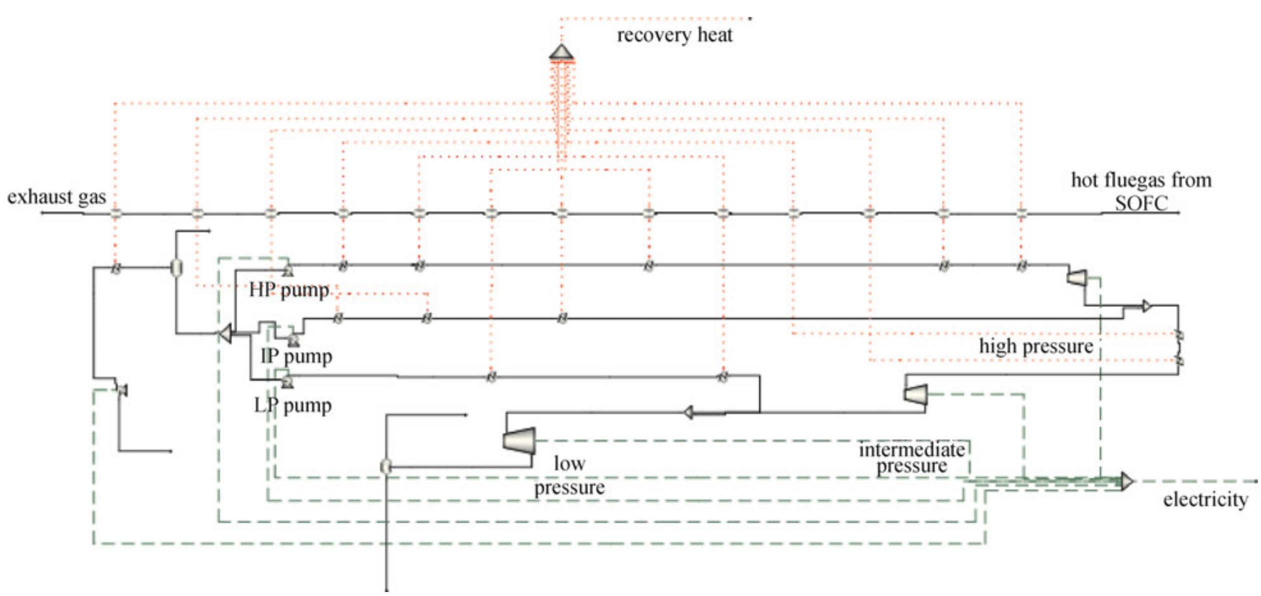

Fig. 4 Modeling of HRSG for steam turbine

efficiency for each stage are calculated. The overall mechanical efficiency for the turbine is estimated using Ref. [15].

The presence of wet vapor at the exhaust means the COMPR block cannot be used to simulate the final stages of the LP section since this block cannot deal with wet vapor with a substantial liquid content. Therefore, the HEATER block, which is normally used to simulate heaters, is modified to simulate these stages. The modified HEATER block calculates and sets the HEATER block exit temperature to that obtained if the expansion is isentropic through the same pressure ratio. The net work output is then set to a value equal to the product of the heat output from the HEATER block and two "efficiency factors." These efficiency factors include correcting for irreversible expansion, which is the same as the stage isentropic efficiency, and correcting for mechanical and generation losses, which is the same as turbine mechanical efficiency.

5 Results

The SOFC inlet temperature for this analysis is assumed 750°C, while the output temperature is 815°C. The electrolyte of the SOFC operates at 600°C–1000°C, at which point the ionic conduction by oxygen ions takes place. Table 1 shows the two different inputs set for the simulation and the mole percentage of fuel cell inlet gas. In simulation A, fuel flow is 80000 kg/h and airflow rate is at 68038 kg/h. For simulation B, they are 100788 kg/h and 85366 kg/h, respectively. The SOFC simulation is considered a pressurized model. Therefore, the ejector pressure ratio is selected as 3 for simulation A and 4 for simulation B.

The Aspen Plus flow sheet of this case is presented in Fig. 3. The stream properties for the SOFC simulation model are documented in Table 2. As temperature, pressure, and mass flow play vital roles in thermodynamic simulation, only these parameters are shown in the table. Figures 5 and 6 show the variation of mole percentage for syngas input, air inlet and anode, cathode outlet in simulations A and B, respectively. Of these two simulations (A and B), simulation A was selected to be used for further simulation, as it is more comparable with the literature value. Table 3 shows the output of the parameters of simulation A, especially for the SOFC input and output streams. The temperature output from the cathode is almost at 815°C, while the pressure is around 127.6 kPa. Vapor friction is almost the same for all streams.

The results of the model primarily constitute the total cell balances and cell internal profiles for any relevant thermodynamic or electrochemical variables. The results of the comparison documented in Table 3 confirm that the system can be improved by operating the SOFC at the specified temperature, pressure, and flow rates. Enthalpy generation from the anode and cathode is used to calculate the SOFC efficiency, as shown in Table 3. The exhaust gas from the SOFC is utilized by the HRSG to produce hot steam for the steam turbine.

Steam input and output data for the different blocks of HRSG simulation by Aspen Plus vary. The temperatures are calculated by Aspen Plus from the pressures and flow rates supplied to the model. The numbers show that the results generated using Aspen Plus simulations are consistent with the operating data. Figure 7 shows the temperature difference on various parts of the HRSG for gas and steam. The HRSG optimum design in the actual technology is based on the concepts of pinch-point and

Table 1 Data for model calibration

parameters	simulation A	simulation B
operating pressure/kPa	128	134
fuel mass flow/($kg \cdot h^{-1}$)	80000	100788
air mass flow/($kg \cdot h^{-1}$)	68038	85366
cell voltage/V	0.75	0.639
cell inlet fuel temperature/°C	750	650
cell inlet air temperature/°C	550	550
ejector pressure ratio (p_{fuel}/p_{SOFC})	3	4
cold and hot stream temperature difference/°C	10	10
fuel composition at cell inlet (mole percentage)	**simulation A**	**simulation B**
H_2O	10	12.5
H_2	24.6	18.7
CO	58.2	53.6
CH_4	6	2.6
CO_2	1.2	11.9
N_2		0.7
O_2		0

Table 2 Steam properties for SOFC simulation model

steam	temperature/°C	pressure/kPa	mass flow/($kg \cdot h^{-1}$)
syngas	700	134	80000
air	550	131	68038
2	1081.669	403.3433	79605.46
3	704.4444	110.3161	79605.46
4	552.0485	82.7371	265351.53
5	454.4444	82.7371	265351.53
6	486.9348	82.7371	265351.53
8	486.9347	103.4214	121961.14
10	826.2416	393.0012	68038.85
11	537.7778	137.8951	68038.85
12	1377.344	137.8951	68038.85
13	1655.109	13.7895	147644.32
14	826.6667	82.7371	147644.32
16	921.1111	134.2104	25683.18
17	1382.899	13.7895	147644.32
27	486.9347	103.4214	185746.1
28	980.6423	115.3141	42355.68
ANDOUT	486.9348	103	307707.21
CATOUT	815.5556	128	25683.18

Table 3 Data of Aspen Plus simulations

ASPEN stream name	syngas	air	ANDOUT	CATOUT
flow/($kg \cdot h^{-1}$)	80000	68038	265351.533	67052.8547
temperature/°C	750	550	486.9	815.6
pressure/kPa	128	128	103.4	127.6
enthalpy/($MMkcal \cdot h^{-1}$)	——	——	−218.95543	11.72038
mole flow	syngas	air	ANDOUT	CATOUT
H_2O/($kmol \cdot h^{-1}$)	396.2408	37.7673	0	37.7673
H_2/($kmol \cdot h^{-1}$)	974.7525	0	4569.978	7.27E-08
CO/($kmol \cdot h^{-1}$)	2306.122	0	6366.269	0
CH_4/($kmol \cdot h^{-1}$)	237.7445	0	792.4817	0
CO_2/($kmol \cdot h^{-1}$)	47.5489	0	1479.299	0
N_2/($kmol \cdot h^{-1}$)	0	1870.168	0	1870.168
vapor fraction	1	1	1	1

approach point, which govern the gas and steam temperature profile. Figure 8(a) shows that the temperature flow of high-pressure water flow increases to a certain amount and then suddenly decreases due to compression. Figure 8(b) and (c) represent the temperature for intermediate- and low-pressure steam flow, respectively. For both cases, the temperature gradually increases. These figures show the heat rate through the different components of the HRSG. High-pressure superheater exit temperature from the HRSG is almost at 538°C, while temperature is at 309°C and 131°C for IP and LP superheater outlets, respectively. Other related output results from the HRSG and steam turbine are given in Table 4. Although the pinch-point temperature is different in each case, the approach temperature difference is the same for both HP and IP cases.

Vapor fraction for both HP and IP sections is 1. Pressure for the HP section is 9570 kPa, while that for the IP section is only 1952 kPa and the LP section is only 392 kPa. By utilizing Eqs. (6)–(11), the steam turbine efficiency can be measured, as shown in Table 4. The net efficiency for the steam turbine is almost 35%. Each turbine (HP, IP, and LP) work can be measured by Aspen Plus simulation, as shown in Table 4.

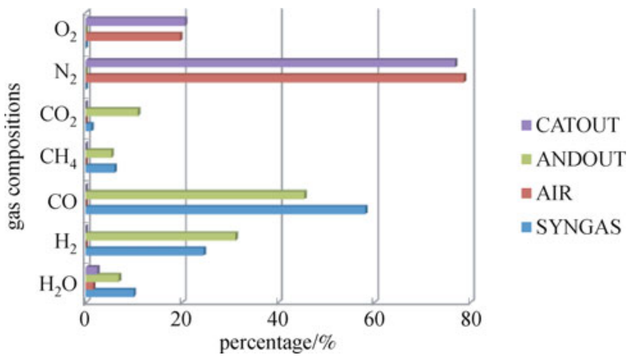

Fig. 5 Percentage of different components for simulation A

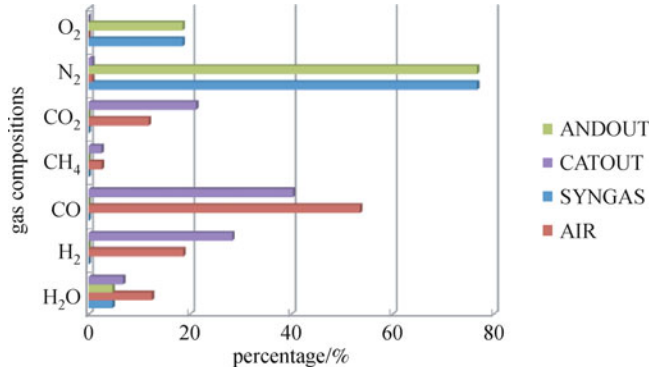

Fig. 6 Percentage of different components for simulation B

Table 4 Triple pressure HRSG-ST output

parameters	HP	IP	LP
superheater temperature T_{sh} /°C	538	400	180
evaporator temperature T_{eva}/°C	309	217	150
economizer temperature T_{eco}/°C	131	130	130
pinch temperature T_{pp}/°C	27	23	44
approach temperature T_{app}/°C	10	10	——
stack temperature T_{stack}/°C		105	
pressure/kPa	9570	1952	392
exit steam quality	1	1	0.9513
turbine work $W_{turbine}$/MW	35.553	45.610	27.041
net work W_{net}/MW		108.204	
net turbine efficiency η_{net}		35.02	

6 Model validation

The developed model was validated against published data for the NETL 300 MW IGFC combine cycle SOFC stack operating on coal [16]. Table 5 shows the comparison between the simulated results and those from literature for the SOFC. Operating pressure is higher than the value in the literature and the reforming percentage is 30, which may affect the fuel utilization factor. SOFC efficiency is measured by Eqs. (1)–(5) using simulation results; it can convert 95% of DC to AC.

As in this model, water circulation is not involved, thus the percentage of H_2O in the anode outlet gas composition is lower than that from the literature (Fig. 9). H_2, CO, and CH_4 values are higher than the compared values, indicating that this output composition can be utilized by the HRSG for better performance.

The overall performance of the plant is compared with the value from the literature, as shown in Table 6. Power generation from the SOFC model for this simulation is lower than that from the literature because of the lower percentage of methane gas from the syngas. In the literature, catalytic gasification system was used instead of normal gasification system. However, the power output from the steam turbine is higher in terms of simulated results. The output gas from the SOFC, which contains higher percentage of CO and H_2, was utilized by the HRSG to drive the steam turbine.

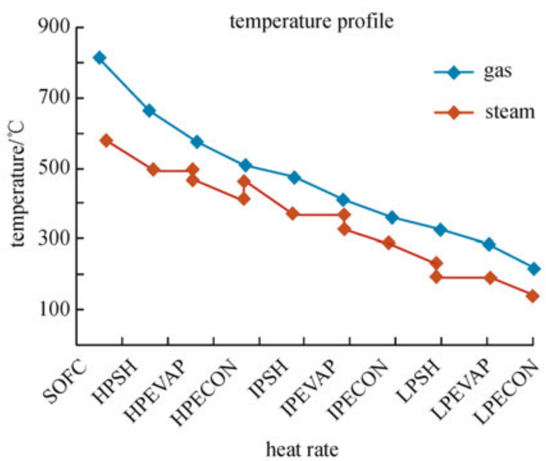

Fig. 7 Temperature profile builds on simulation results

Table 6 shows that the power generated from the steam turbine are at 108.204 MW, which is almost three times

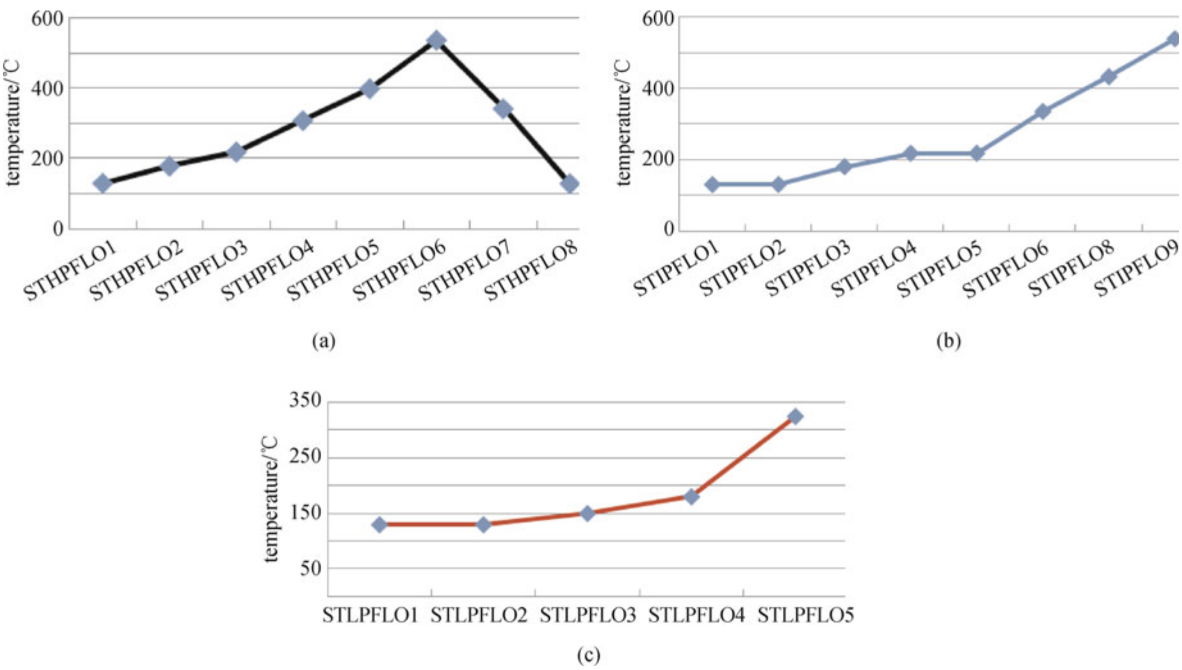

Fig. 8 Temperature profile for
(a) HP steam; (b) IP steam; (c) LP steam

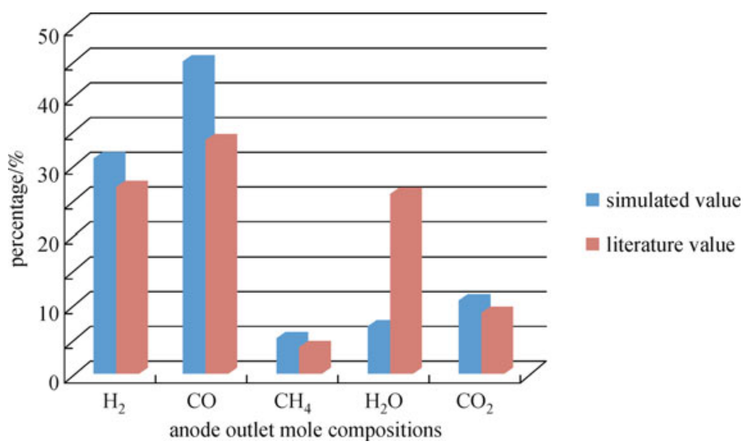

Fig. 9 Comparison of Anode outlet composition

that of the value from the literature. The loss from the HRSG feed water pump is superior in the simulation because of the higher water flow rate. Some losses such as in coal and slag handling were taken from the referenced article from where syngas properties were taken. In terms of total loss, the simulated value is almost 5.4 MW higher than the compared values. Excluding the losses, the total production is 41.88 MW more for the simulated design. However, net efficiency is slightly higher in literature as it has more electricity produced from the SOFC. One of the reasons for this is that in the model from the literature, the water exhaust was recycled from the anode output.

7 Conclusions

In the IGFC configuration, power is generated by both the fuel cell and the steam cycle. The fuel cell is the most efficient energy conversion device in the cycle. Therefore, system efficiency (48.28) was improved compared with other convention power plants, as energy conversion in the SOFC is optimized in terms of fuel utilization and overpotential reduction.

A simulation model of the SOFC stack was developed using Aspen Plus. It is flexible enough for industrial uses and capable of predicting system performance under

Table 5 Comparison of simulation data with data from literature

parameters	simulation	literature
single cell voltage/V	0.72	0.69
current density/($A \cdot m^{-2}$)	1800	–
operating pressure/psia	19.5	18
air intake rate/($lb \cdot h^{-1}$)	68038	78500.6
pre-reforming percentage/%	30	–
compressor pressure ratio	3	–
fuel mass flow/($lb \cdot h^{-1}$)	80000	96514
cathode exhaust gas composition (mole)/%	N_2 = 76.9, O_2 = 18.56, H_2O = 4.18, H_2 = 0.36	N_2 = 80, O_2 = 18, H_2O = 2
fuel utilization/%	72	–
air utilization/%	18	–
system fuel effectiveness with IGFC/%	86.6	–
inverter efficiency/%	95	92
gross AC efficiency (LHV)/%	52	51.5
SOFC efficiency/%	59	

Table 6 Comparison of whole power output with data from literature

power production summary	simulation results	literature results
SOFC power/MW	238.546	264.575
steam cycle power/MW	108.204	34.859
total	346.75	299.470
auxiliary power summary	simulation results	literature results
cathode blower/MW	8.550	13.760
syngas recycle compressor	1.160	1.354
ASU compressor	9.440	7.005
gasifier O_2 compressor	5.140	6.254
HRSG feed water pump	3.030	0.942
coal input loses (handling, milling, and slurry pumps)	2.125	1.223
slag handling, and dewatering	0.617	0.534
condensate pump	0.153	0.0765
circulating water pump	0.570	0.125
cooling tower fan	0.980	0.393
Selexol auxiliaries	1.595	1.431
miscellaneous balance of plant	0.436	0.985
transformer loss	2.080	0.976
CO_2 compression	15.6	16.45
total	51.476	46.08
net total power	295.27	253.39
AC/DC inverter efficiency/%	97	
net efficiency/%	48.28	49.4

various operating conditions. The total electricity production from the SOFC is almost 238.546 MW for this IGFC system. The SOFC simulation was made for two different coals, and simulation A was selected for further simulation, as it has better output results for the HRSG operation.

For the HRSG, the following conclusions are reached.

1) Since the live steam temperature of the steam turbine is restricted by the exhaust gas temperature from the SOFC and the temperature difference at pinch point, the steam subsystem matching the high exhaust temperature can achieve higher steam parameters.

2) HRSG simulation was completed in complex configuration with triple pressure with reheat. The plotted temperate profile for the HRSG using the simulation results shows the actual temperature profile graph, which makes the model better for validation. The power generated from the steam turbines using the steam from the HRSG is 108.204 MW.

The results of the cases presented in the result section illustrate how an IGFC system has more efficiency benefits over other advanced power generation technologies. If advanced fossil energy research goals in the areas of coal gasification and solid oxide fuel cell development are met, this study demonstrates an IGFC combined cycle of 48.28% efficiency.

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Paper 7

Conceptual Design of an Integrated Hydrothermal Liquefaction and Biogas Plant for Sustainable Bioenergy Production.

Hoffmann, J. Rudra, S.; Rosendahl, L; Toor, SS; Nielsen, JBH.

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Conceptual design of an integrated hydrothermal liquefaction and biogas plant for sustainable bioenergy production

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HIGHLIGHTS

- ▶ Initial process modelling on a combined biogas and hydrothermal liquefaction plant.
- ▶ The plant produces biofuels from low value biomass feedstock, like cattle manure.
- ▶ Mass and energy balances for two biogas yield scenarios have been done.
- ▶ Aspen Plus and model compounds for biomass and biofuel have been used.
- ▶ 52–63% of the input biomass energy to the plant is recovered in the liquid biofuel.

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ABSTRACT

Initial process studies carried out in Aspen Plus on an integrated thermochemical conversion process are presented herein. In the simulations, a hydrothermal liquefaction (HTL) plant is combined with a biogas plant (BP), such that the digestate from the BP is converted to a biocrude in the HTL process. This biorefinery concept offers a sophisticated and sustainable way of converting organic residuals into a range of high-value biofuel streams in addition to combined heat and power (CHP) production. The primary goal of this study is to provide an initial estimate of the feasibility of such a process. By adding a diesel-quality-fuel output to the process, the product value is increased significantly compared to a conventional BP. An input of 1000 kg h^{-1} manure delivers approximately 30–38 kg h^{-1} fuel and 38–61 kg h^{-1} biogas. The biogas can be used to upgrade the biocrude, to supply the gas grid or for CHP. An estimated 62–84% of the biomass energy can be recovered in the biofuels.

1. Introduction

The need for renewable and sustainable energy sources is high because of a number of factors: the increase in global energy demand, depletion of conventional resources, climate issues and the desire for national/regional energy independence. In 2010, fossil fuels still accounted for 87% of global and 79% of EU primary energy consumption (BP, 2011). Liquid fuels from biomass are essential to meet the imposing challenges of energy and climate (U.S. Energy Information Administration, 2011) due to their carbon neutrality. Marine, aviation and heavy land transport in particular are not likely to become electrified within the next few decades, and for these vehicles, the challenge becomes one of supplying them with suitable drop-in replacement fuels derived from biomass. Because biomass will also be a prime feedstock for a wide range of chemical, nutritional and pharmaceutical products, it will become a limited, high-cost commodity. Therefore, for liquid biofuels to be produced in bulk, it is necessary to identify eligible low-value organic streams such as animal manure, agro-industrial waste and sewage sludge.

For this to occur, the identification of suitable combinations of feedstocks and conversion processes that ensure high process and conversion efficiency and the sustainability of the biomass in the fuel conversion process are critical. The latter is especially important because the energy from fossil fuels used during the biomass conversion process has to be considered in the carbon footprint. The responsible use of resources and minimisation of fossil energy inputs to the process should be targeted. Only an efficient and sustainable process will be commercially compatible and have the capacity to endure. Appropriate process integration and optimisation are the best methods to achieve this.

This work focuses on developing a process design concept for the sustainable production of drop-in biofuels from organic waste streams. In particular, the process design integrates a biochemical (biogas plant – BP) and a thermochemical (hydrothermal

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Nomenclature

BP	biogas plant
DM	dry matter
HPU	hydrogen production unit
HTL	hydrothermal liquefaction
LHV	lower heating value
UU	upgrading unit

liquefaction – HTL) biomass conversion process, with the HTL feeds resulting from the waste stream of the BP. The end-products of the integrated process are a range of biofuels (biogas, biocrude or upgraded biofuel) that can be used for transportation as well as for combined heat and power (CHP) production. Fig. 1 shows a schematic overview of the plant.

1.1. Biogas

In a biogas plant, organic materials, such as animal manure, energy crops or industrial organic sludge, are anaerobically digested to produce biogas in airtight reactors. Through this decomposition, organic bound carbon in the biomass slurry is converted primarily into a mixture of CH_4 and CO_2 Two operation modes are used: mesophilic and thermophilic digestion. Mesophilic plants digest at 35–40 °C, and thermophilic plants operate at 50–60 °C. The biogas produced is mainly used for CHP production, but it can also be used directly or purified to yield CH_4 for other purposes. The leftover product, the digestate, is commonly used as fertiliser on farm land. Waste biomass such as animal manure is highly available in the European Union and is thus a very interesting feedstock. In Denmark, 46 million tonnes of waste biomass are produced annually, and Germany and France produce 232 and 300 million tonnes, respectively (Holm-Nielsen and Oleskwicz-Popiel, 2008).

1.2. Issues regarding degassed manure

Normally, the digestate is used as fertiliser and distributed on fields, closing the nutrient and carbon cycle. Thus, the disposal time of the digestate has to be scheduled based on weather conditions. Most countries restrict the spreading of digestate during winter, requiring manure to be stored in facilities during that time. As biogas production has increased, storage and disposal issues have become more critical (Lootsma, 2008).

Work carried out by Döhler and Schliebner (2006) shows that if the transport distance of the digestate exceeds 5–10 km, the cost for transport and spreading of the digestate on the field are higher than the fertilising value of the digestate. Another problem is that the substrate inputs to biogas plants are normally transregional, so recirculation of nutrients in the immediate neighbourhood of the plant is not feasible as a method to limit transport costs because the nutrition load exceeds the absorption capacity of the agricultural land. Furthermore digestates may contain heavy metals and other organic pollutants, which are not biologically degradable after spreading and will accumulate in the soil. If the digestate cannot be spread on the field due to economic limitations or spreading restrictions and limitations, high costs for storage will arise, which will influence the agricultural economy enormously. Conditioning, spreading and storage of digestate depending on the process used amounts to 7–14 € m^{-3} of digestate (Döhler and Schliebner, 2006). Processing the digestate from a biogas plant directly in a coupled hydrothermal liquefaction unit is therefore advantageous.

Another significant issue encountered when handling digestate from animal manure is sanitation. The intestinal fiora of animals naturally contains bacteria, viruses and parasites, and zoonotic agents can cause infections in humans such as influenza and salmonella. Animal pathogens can cause animal disease epidemics such as swine fever and foot-and-mouth disease (Baggesen, 2007). Treatments for the high-risk manure from the 16 million tonnes (Holm-Nielsen and Oleskwicz-Popiel, 2008) of animal materials that are excluded from the food chain in the EU-27 each year include steam sterilisation at a temperature of 130 °C for 20 min, and low-risk manure demands pasteurisation at a temperature of 70 °C for 1 h. Biogas plant owners are obliged to instal a pasteurisation/hygenisation unit, including measurement and control devices to treat the high or low risk feed. This extra unit results in higher investment and operation costs for the plant. If the digestate were converted in a hydrothermal liquefaction process at

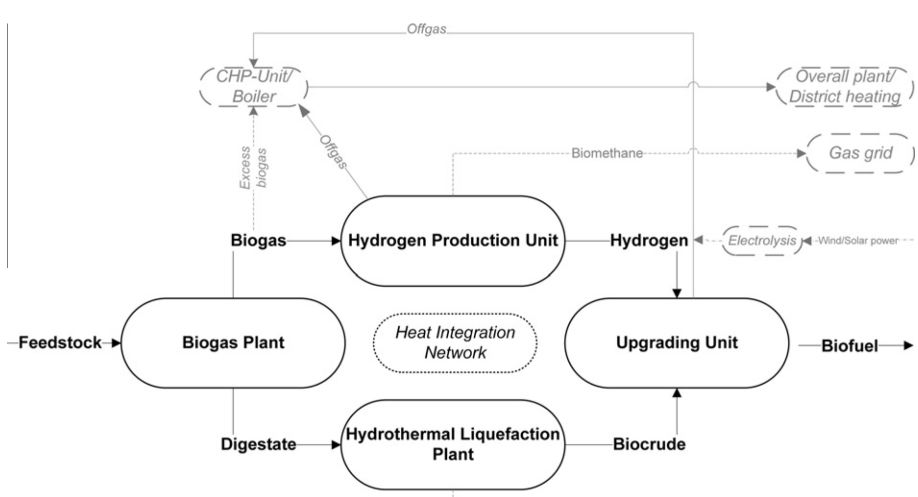


Fig. 1. Schematic overview of the conceptual process design.

temperatures of 280–360 °C, the hygenisation step of the feed would become redundant, and costs could be reduced.

1.3. Process description

The digestate obtained from anaerobic digestion (compare Section 1.1) is further converted using hydrothermal liquefaction. During hydrothermal liquefaction (HTL), wet biomass feedstock is converted at medium temperatures and pressures (280–360 °C, 180–300 bar) into a liquid biomass fuel, referred to as biocrude hereafter. The reaction time is normally 10–60 min, and catalysts are often used. In the literature, biocrude mass yields are reported as 6–10% of the biomass input mass and 34% of the dry matter in the feed, depending on the feedstock used (Toor et al., 2012; Hammerschmidt et al., 2011). By-products of the HTL process are a solid fraction containing nutrients, minerals and metals; a water fraction containing low amounts of soluble organics; and a gas fraction, mostly consisting of CO_2. For biocrude to be used as a drop-in transportation biofuel, upgrading the crude is necessary. The higher oxygen content in the biocrude leads to undesirable properties. The properties that most negatively affect biocrude quality are low heating value, incompatibility with conventional fuels, solids content, high viscosity, incomplete volatility, and chemical instability (Huber et al., 2006). To obtain a diesel-like fuel from the biocrude, the oxygen content needs to be lowered. This can be achieved through hydrotreating of the crude. In this process, the biocrude is pressurised with hydrogen in the presence of a catalyst. Biocrude from hydrothermal liquefaction normally contains approximately 5–10 wt.% oxygen (compare Table 2).

The gas products from the biogas plant (mainly CO_2 and CH_4) can be used to generate heat and electricity for the plant, upgraded and fed to the gas grid or steam-reformed to H_2 and used for further hydrotreating of the biocrude for conversion into diesel quality fuel. Offgas from the steam reforming and upgrading units can also be used for internal heat and the power supply. For end-use applications such as marine transport, the biocrude can be used with little or no upgrading. Waste water from the hydrothermal liquefaction unit, can be used for fertiliser purposes and integrated to the heat recovery network of the plant.

This proposed coupling and integration of several processes offers multiple advantages over an individual, stand-alone biogas plant. In the following sections, the simulation of such a plant is described and evaluated.

2. Methods

In this section, the simulation of an integrated plant in Aspen Plus is described and evaluated.

2.1. Process development and calculation method

For simulation of the overall process, Aspen Plus V 7.3 is used. As an initial effort in simulation of this biomass conversion process, the overall process is divided into four independent sections: anaerobic biomass digestion (biogas plant), hydrogen production, hydrothermal liquefaction, and upgrading of the biocrude. The energy demand of a separation utility has been neglected for every unit. Fig. 2 shows the design of the overall plant and the mass and energy flows between the independent units.

In Aspen Plus, the Soave-Redlich-Kwong (SRK) cubic equation of state for all thermodynamic properties is used for the simulation. The biomass input and the digestate are modelled as non-conventional solids using two special models named HCOALGEN and DCOALIGT. These models are designed for coal-derived materials. HCOALGEN models the enthalpy of the biomass and digestate, whereas DCOALIGT is used to model the density of the components. HCOALGEN requires input of the ultimate, proximate and sulphanate analysis of the component. The HCOALGEN model includes a number of different correlations. For the heat of combustion, the heat of formation and the heat capacity, the Boie correlation, a heat-of-combustion-based correlation and the Kirov correlation are used, respectively, based on the entered elemental attributes of the components. For the calculations, elements are assumed to be in their standard states (298.15 K and 1 atm). The

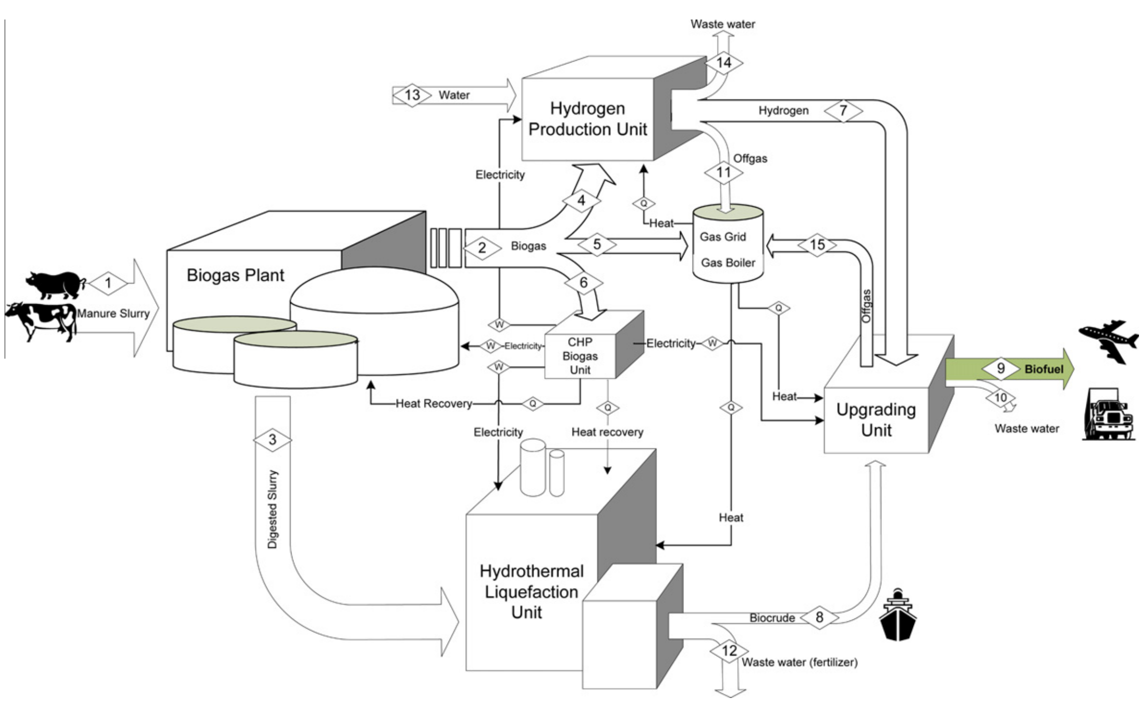


Fig. 2. Mass and energy flow of the overall plant.

Table 1
Proximate and Ultimate analysis of manure substrate and thermophilic digestate (Otero et al., 2011).

	Fresh manure	Thermophilic digestate
Proximate		
Volatiles (%)	62.3	55.5
Fixed carbon (%)	17	18.8
Ash (%)	20.7	25.7
Water content (%)[a]	7	6.8
Ultimate		
C (%)	37.9	35.8
H (%)	10.1	9.5
N (%)	3	3.2
S (%)	0.3	0.3
O (%)[b]	28	25.5
Heating value (MJ kg^{-1}) (dry)	15.64	14.71
Heating value (MJ kg^{-1}) (slurry)	2.69	2.26

[a] Water content of oven dried sample.
[b] Calculated by difference.

Table 2
Oxygen content of different biocrudes.

	Refs.	Feedstock	Oxygen in mixture (wt.%)
Biocrude from HTL	Toor et al. (2012)	WDGS	5.6 ± 0.4
	Zhong et al. (2002)	Microalgea	25.08
	Hammerschmidt et al. (2011)	Organic waste streams	10
	Elliott and Schiefelbein (1989)	Not specified	16.3
Model-biocrude 80 wt.% phenol 20 wt.% hexadecanoic-acid		Digestate	16.1
Upgraded biocrude	Furimsky (2000)		0.0–0.7

DCOALIGT model uses ultimate and sulfanate analysis and is based on equations from the IGT (Institute of Gas Technology) (Aspentech, 2011).

2.2. Model compounds

2.2.1. Biomass substrate and digestate

As mentioned above, Aspen Plus requires ultimate, proximate and sulfanate analysis of the biomass input and digestate. All sulphate is considered to be organic sulphur.

Table 1 shows the ultimate and proximate analyses used for this simulation, with values taken from the literature (Otero et al., 2011). Reactors have been modelled on yield results or stoichiometries, using the RYield or RStoic Aspen Plus reactor models, respectively. Aspen Plus calculates energy and mass balances for the complete process of converting biomass to biofuel. Methods for each unit are described in the following sections. The results make it possible to evaluate the potential usefulness and sustainability of the system.

The lower heating value (LHV) of the substrate manure and digestate is calculated in the ultimate analysis by using the Boie correlation (Eq. (1)) (Boie, 1957).

$$LHV_{Boie} = 34.8C + 93.9H + 6.3N + 10.5S - 10.8O - 2.44H_2O \quad (1)$$

The dried biomass substrate sample and digestate have calculated heating values of 15.64 and 14.71 MJ kg^{-1}, respectively. Their heating values in the wet manure slurry is 2.69 and 2.05 MJ kg^{-1} for the digestate from scenario 1 and 1.8 MJ $kg^{-1}$for the digestate from scenario 2, respectively.

2.2.2. Biocrude

The biocrude is modelled as a mixture of 80 wt.% phenol and 20 wt.% hexadecanoic acid, leading to an oxygen content of 16.1 wt.%. This composition is based on GC/MS analysis of biocrudes from hydrothermal liquefaction (Toor et al., 2012; Elliott and Schiefelbein, 1989).

2.3. Biogas plant

The amount of biogas obtained from the manure feed depends on several factors: the dry matter content of the slurry, the origin of the slurry and the conditions and reaction time in the digester. For this model, the input to the biogas plant is assumed to be 1000 kg h^{-1}. The digestion process used in this study works under thermophilic conditions; thus, a digester temperature of 51 °C is used in the simulation. The values and properties for the substrate and digestate are taken from Otero et al. (2011). The biomass utilised in the biogas plant is cattle manure plus bedding material with a total dry matter (DM) content of 17.2 wt.%. The total DM consists of 82.7 wt.% volatile solids (VS). The proximate and ultimate analyses used to model substrate and digestate in Aspen Plus can be found in Table 1. Simulations have been performed on two different biogas yield scenarios. Scenario 1 addresses a low yield of biogas: 0.26 m^3 kg^{-1} VS, a value obtained from the laboratory-scale studies of Otero et al. (2011). Scenario 2 assumes a higher biogas yield of 0.45 m^3 kg^{-1} VS, which is a value normally used as a reference when planning biogas plants using cattle manure plus bedding material (Anspach, 2009). The biogas is modelled as 62 vol.% CH_4 and 38 vol.% CO_2. For both simulations, biomasses with the same proximate and ultimate analyses and DM content in their substrates are used.

The digester is modelled as a RYield reactor in Aspen Plus. It is assumed that no water vaporises during the digestion process. Thus, the dry matter content of the digestate can be calculated using Eq. (2).

$$(DM_{biomass} m_{biomass} - m_{biogas})/m_{digestate} = DM_{digestate} \quad (2)$$

Fig. 3 shows the flowsheet configuration used in Aspen Plus. The stream numbers refer to the numbers used in Fig. 2.

A portion of the biogas from the digestion process is sent to the upgrading facility and is used in a CPH unit before eventually going to a gas boiler. The electrical efficiency of the CHP unit is assumed to be 39%. The thermal efficiency is assumed to be 52%, and the thermal efficiency of the gas boiler is set at 98%.

2.4. Hydrothermal liquefaction unit (HTL)

In scenario 1, 962.11 kg h^{-1} digestate from the biogas plant is sent to the hydrothermal liquefaction unit, where it is converted to biocrude. In the scenario 2, 938.43 kg h^{-1} is sent for further conversion. The HTL reactor is modelled as a RYield reactor. Conversion conditions (T = 330 °C and p = 250 bar) in the HTL reactor and biocrude yields are taken from Hammerschmidt et al. (2011), and full conversion of the digestate is expected. It is assumed that exothermic and endothermic reactions are balanced during the biomass to biocrude conversion. The designed Aspen flowsheet is shown in Fig. 4. The recycle loop is neglected in these preliminary process studies, but using a recycle loop would be expected to lower the heating duties.

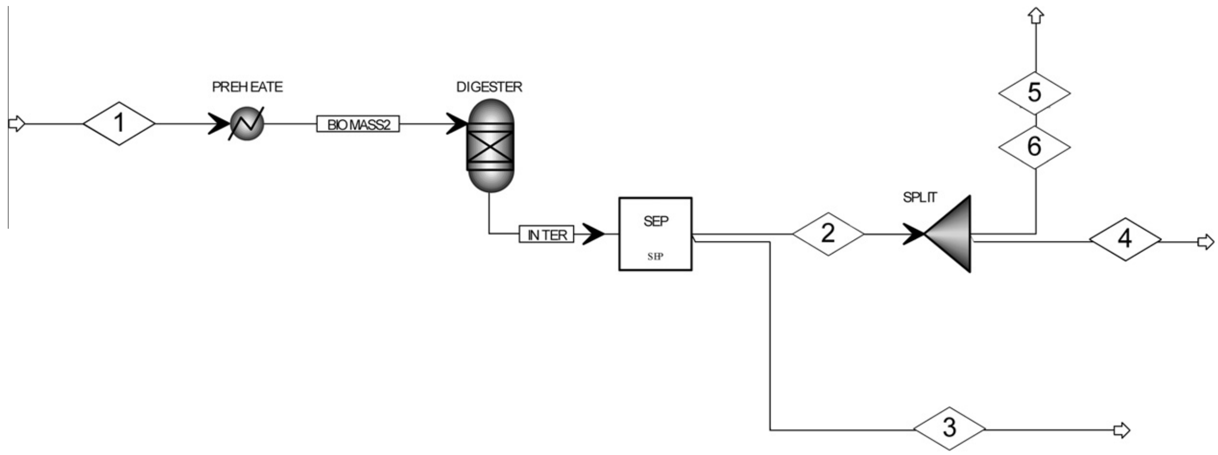


Fig. 3. Flowsheet of the biogas plant unit.

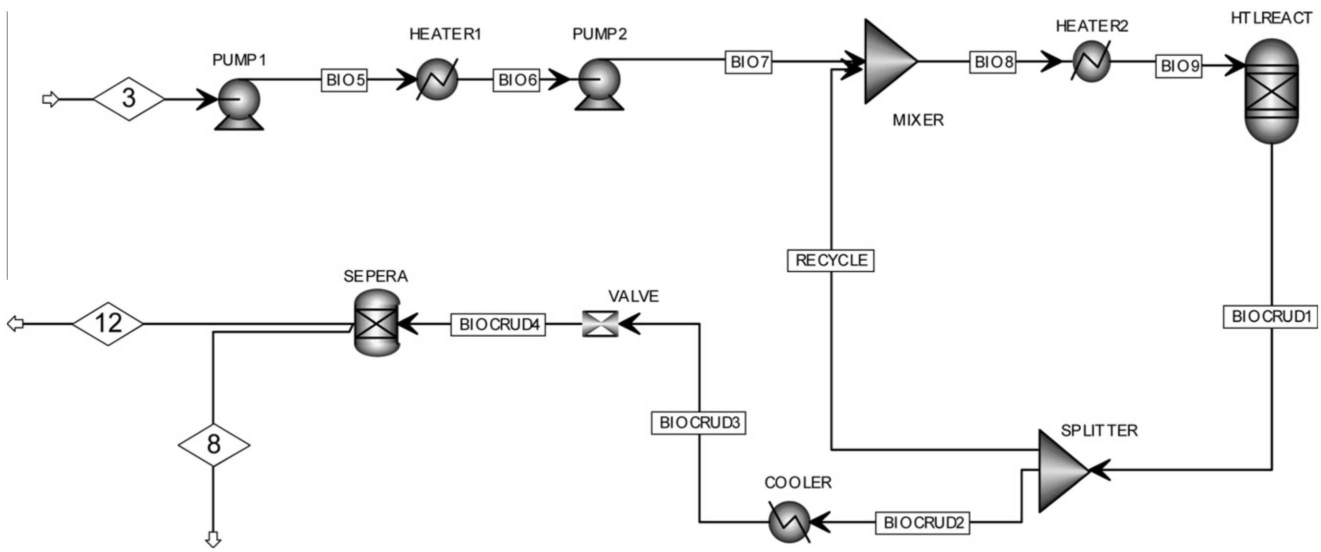


Fig. 4. Flowsheet of the HTL unit.

2.5. Hydrogen production unit (HPU)

The flowsheet used for the simulation of the HPU is shown in Fig. 5. The process is described in more detail below.

2.5.1. Methane recovery

To upgrade the biocrude, hydrogen needs to be produced from part of the biogas stream. Thus, the biogas components are separated using a membrane separator. A membrane module described by Deng and Hägg (2010) for biogas separation results in a recovery of 99% CH_4. This setup consists of a recycle process, two membrane units with different feed pressures and several compressors and heat exchangers. However, the membrane module in this simulation is simplified to consist of one multistage compression series and one membrane unit. This is shown in the flow sheet in Fig. 5. Although this simple membrane setup is not the most efficient in terms of recovering CH_4 (Deng and Hägg, 2010), a CH_4 recovery of 100% is assumed in order to simplify the model. The compression of biogas is modelled with intercooling (C2–C4) to minimise the required compression work. Because the compressor work increases with temperature, it is desirable to compress at low temperatures, so the output temperature from the compressors is set to 291 K. The pressure ratio r_p for each compressor is set to less than 3.5 in the membrane unit on the basis of a previous study (Deng and Hägg, 2010). The inlet temperature of biogas entering the gas separation unit is 51 °C, thus requiring cooling to the operating temperature of 25 °C (Deng and Hägg, 2010).

2.5.2. Methane steam reforming

The pre-treated feed gas (CH_4) is mixed with steam before entering the reforming reactor. The ratio $n_{water}/n_{methane}$ is set to 1.5. The steam methane reforming (SMR) reaction is highly endothermic and catalysed by nickel (Molburg and Doctor, 2003). The conversion of methane is 75%. The stoichiometric reaction is shown in Eq. (3).

$$CH_4 + H_2O \rightarrow 3H_2 + CO \quad (3)$$

Excess steam is added to prevent coke formation in the reactor tank. In the reactor tank, the gas mixture is channelled through nickel catalysts. The temperature inside the reactor varies from to 750 to 850 °C (Molburg and Doctor, 2003). The gas mixture leaving the SMR unit is cooled and then channelled to the high temperature shift tank (HTS) before going to a low temperature shift tank

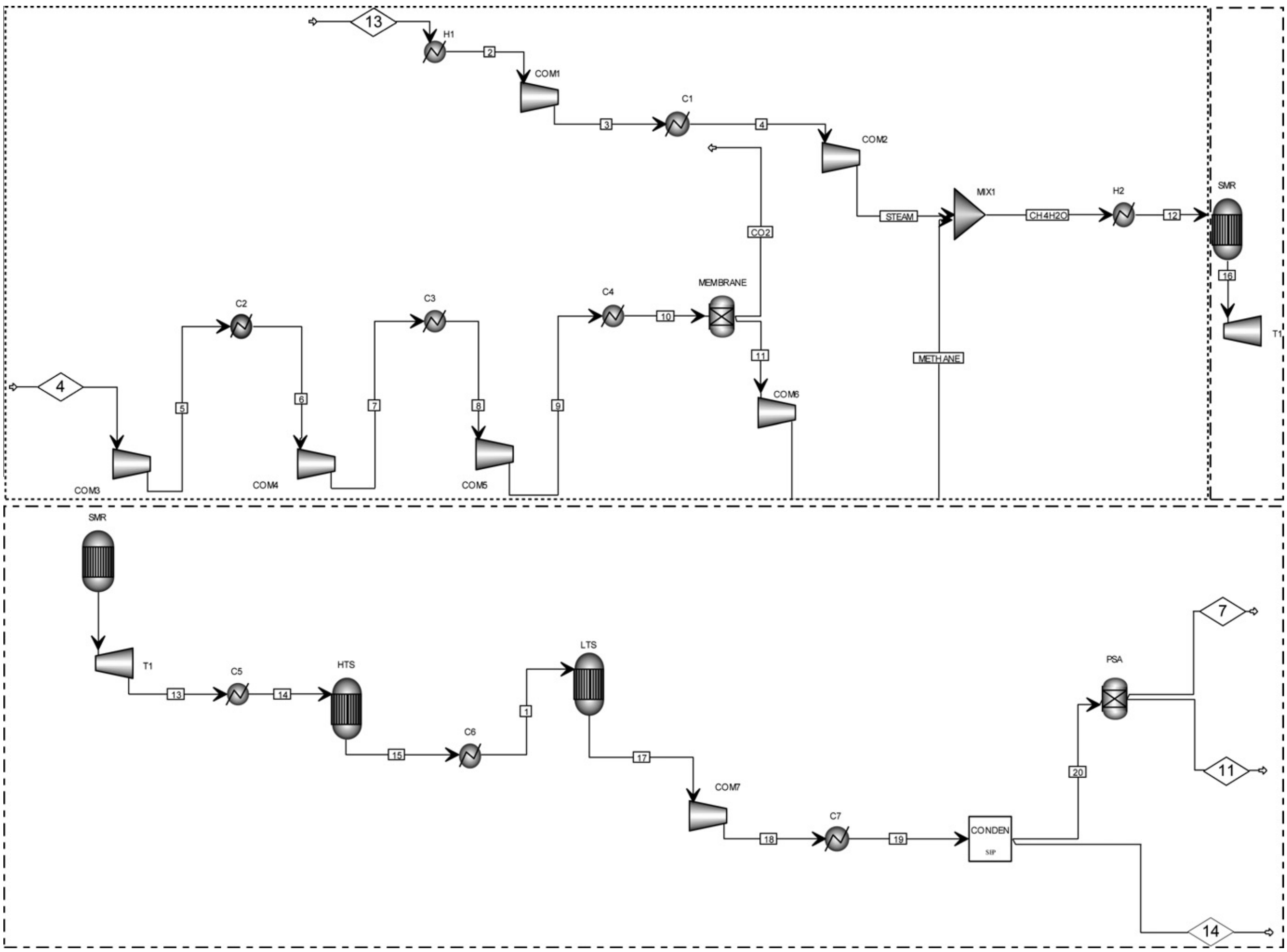


Fig. 5. Flowsheet of the HPU (dotted lines show the methane recovery part of the unit whereby the dashed line show the steam reforming part of the unit).

(LTS), where the exothermic water-shift reaction occurs (Eq. (4)). The process temperatures are 350 °C and 190–210 °C for the HTS and LTS tanks, respectively (Molburg and Doctor, 2003).

$$CO + H_2O \rightarrow CO_2 + H_2 \quad (4)$$

The HTS tank is used to ensure a high reaction rate between CO_2 and steam. However, it is necessary to use the LTS tank to ensure a high conversion rate. The conversion of CO in the HTS and LTS reactor is 90%. Generally, in an HTS tank, an iron-based catalyst is used, and in an LTS tank a copper-based catalyst is used (Molburg and Doctor, 2003).

The purification of hydrogen is performed using pressure swing adsorption (PSA). For simplicity, the PSA unit is represented by a compressor (COM7) and a cooler (C7) in the theoretical model.

2.6. Upgrading unit (UU)

For this simulation, three oxygen-eliminating reactions for the fatty acid model compound have been taken into account. Oxygen atoms can be removed from the carboxylic group of hexadecanoic acid in the form of water by hydrodeoxygenation (R6). In the hydrodecarbonylation reaction, oxygen can be eliminated as CO and water (R7). Hydrodecarboxylation leads to the elimination of a carboxylic group in the form of carbon dioxide (R8). In Table 2, these reactions are listed, along with the conversion rates found in the literature. For reactions R6–R8, reaction rates have been estimated assuming full conversion of hexadecanoic acid.

To keep the process sustainable, hydrogen for the upgrading process is made available through steam reforming of biogas, which is fed to the upgrading unit of the plant. In Fig. 6, the flowsheet configuration in Aspen Plus is shown. Hydrogen and biocrude are being compressed to 80 bar and heated to 80 °C, mixed and sent to the upgrading reactor (UREACTOR). Process conditions are adapted from (Ahmad et al., 2010). The process is run with a molar ratio of $n_{\text{hydrogen}}/n_{\text{biocrude}} = 3$. The end-product biofuel from the model is a mixture containing conventional diesel fuel components: benzene, cyclohexanone, cyclohexane, hexadecane and pentadecane.

3. Results and discussion

In this study, a steady-state system has been modelled to provide an initial model without the potentially complex considerations of dynamics. The process simulation was performed with operating conditions based on data from the literature.

The simulation indicates the feasibility of the conceptual process design. In Table 4, all mass and energy flows of the plant are listed, and the stream numbers refer to the numbers used in Fig. 2 and the Aspen flowsheets for each unit Fig. 3. The results are given for the low- and high-yield scenarios, scenario 1 and 2, respectively. From an input of 1000 kg h^{-1} low-value manure in both scenarios, 36.8 and 30.32 kg h^{-1}, respectively, of high value diesel-like fuel can be produced. The upgraded model biofuel consists of 28.2 wt.% phenol, 26.2 wt.% cyclohexane, 15.7 wt.%

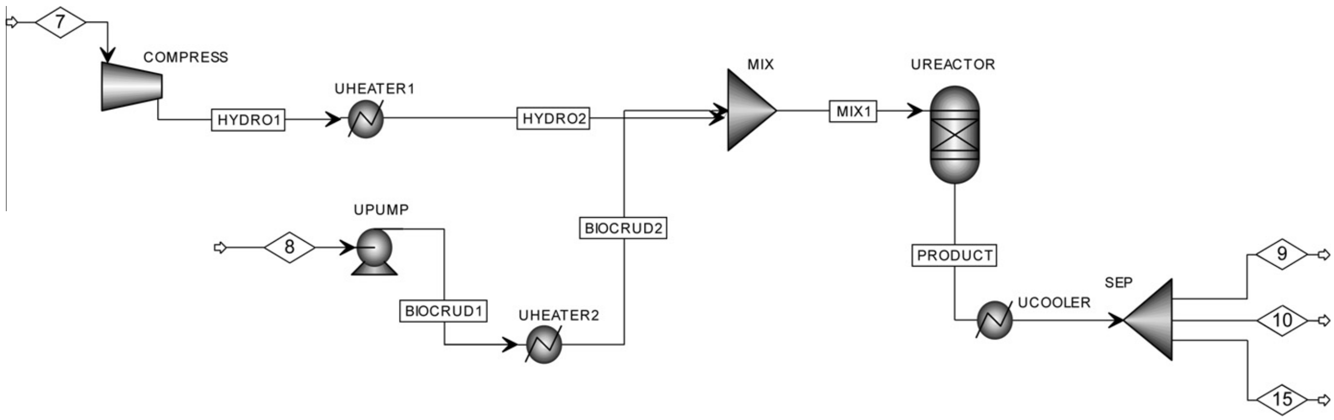


Fig. 6. Flowsheet of the upgrading unit.

Table 3
Overall upgrading process reactions of model compounds (**1**–**5**) adapted from (Ahmad et al., 2010).

Model Compound	Reaction		Conversion[a] (%)	Ref.
Phenol				
Phenols → Benzene	$C_6H_5(OH) + H_2 \rightarrow C_6H_6 + H_2$	(R1)	34	[c]
Phenols → Cyclohexanone	$C_6H_5(OH) + 2\ H_2 \rightarrow C_6H_{10}O$	(R2)	34	[1]
Cyclohexanone → Cyclohexanol	$C_6H_{10}O + H_2 \rightarrow C_6H_{11}(OH)$	(R3)	100	[d]
Cyclohexanol → Cyclohexene	$C_6H_{11}(OH) \rightarrow C_6H_{10}+H_2O$	(R4)	100	[d]
Cyclohexene → Cyclohexane	$C_6\ H_{10} + H_2 \rightarrow C_6H_{12}$	(R5)		[2]
Hexadecanoic acid				
n-Hexadecanoic acid → *n*-Hexadecane	$C_{16}H_{32}O_2 + 3\ H_2 \rightarrow C_{16}H_{32} + 2H_2O$	(R6)	80	[b]
n-Hexadecanoic acid → *n*-Pentadecane	$C_{16}H_{32}O_2 + H_2 \rightarrow C_{15}H_{32} + CO + H_2O$	(R7)	10	[b]
n-Hexadecanoic acid → *n*-Pentadecane	$C_{16}H_{32}O_2 \rightarrow C_{15}H_{32} + CO_2$	(R8)	10	[b]

[a] T = 300 C and p = 80–82 bar catalyst $CoMo\text{-}Al_2O_3$.
[b] Estimated.
[c] Gutierrez et al. (2009).
[d] Senol (2009).

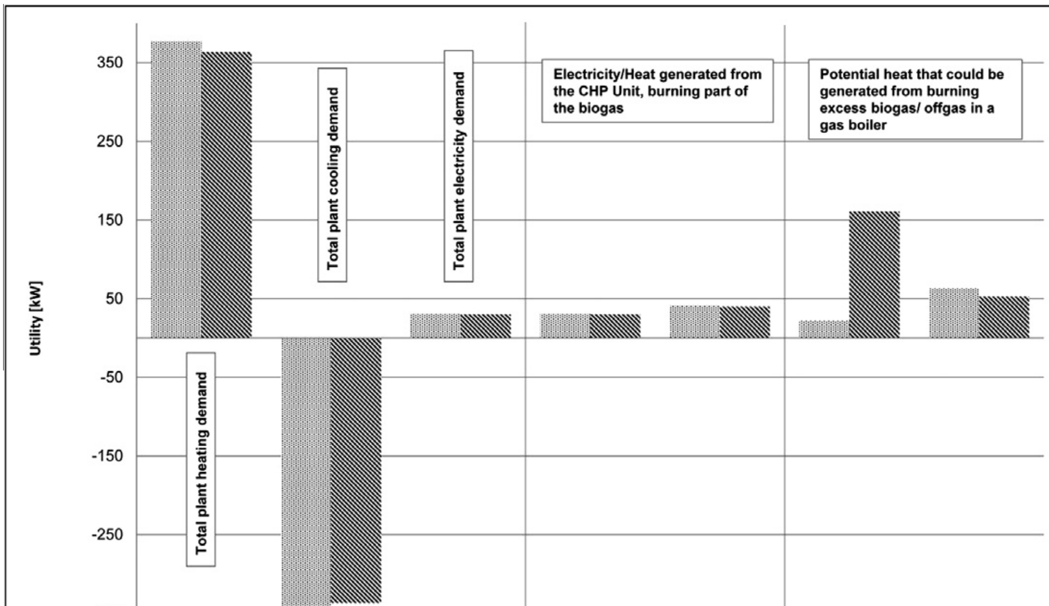
Table 4
Mass- and energy flows of the overall plant.

Stream	*Scenario 1 low gas yield*		*Scenario 2 high gas yield*		Type	Origin	Purpose
	Mass flow (kg h^{-1})	Energy flow (MJ h^{-1})	Mass flow (kg h^{-1})	Energy flow [MJ h^{-1})			
1	1000	2690	1000	2690	Substrate slurry		BP
2	37.88	704.57	61.6	1145.76	Biogas	BP	HPU/CHP Unit/gas boiler/grid
3	962.12	1972.35	938.4	1623.43	Digested slurry	BP	HTLU
4	18.35	465.87	15.3	284.58	Biogas	BP	HPU
5	4.33	80.54	31.59	587.57	Biogas	BP	Gas boiler/gas grid
6	15.2	282.72	14.71	273.61	Biogas	BP	CHP unit
7	2.3	276	1.9	228	Hydrogen	HPU	UU
8	40.96	1645.92	33.73	1214.28	Biocrude	HTLU	HPU
9	36.8	1770.98	30.32	1306.79	Biofuel	UU	End product
10	5.27		4.36		Waste Water	UU	Recycle
11	16	117.43	13.33	97.84	Offgas	HPU	Gas boiler
12	853.93		849.35		Waste water	HTLU	Recycle/fertilizer
13	18.91		15.51		Water		HPU
14	7.44		5.95		Waste water		Recycle
15	1.18	114.88	0.97	94.43	Offgas	UU	Gas boiler

n-hexadecane, 25.4 wt.% benzene, 3.7 wt.% *n*-pentadecane, and 0.8 wt.% cyclohexene, with a density of 0.873 kg l^{-1} and it is estimated to have a heating value of 43 MJ kg^{-1} similar to that of fossil diesel fuel. The net value of diesel-quality fuel obtained equals 327,000 a^{-1} for scenario 1 and 270,000 a^{-1} for scenario 2 at a net selling price for diesel fuel of 0.89 € l^{-1} (See Table. 3).

The utilities of the process are listed in Table 5. Separation steps and pressure drops in the system have been neglected. The heating utility needed is approximately 377 kW for scenario 1 and 363 kW for scenario 2, and the cooling utility is approximately 341 and 337 kW, respectively. The relationship between the cooling and heating utilities illustrates the high potential for process integration and the need for further development of a heat recovery system. Pending this development, the evaluation of the plant is based on the electricity needs for pumps and compressors as modelled. These utilities are covered by burning the remaining biogas (i.e., that which is not used for biocrude upgrading) partially or completely in a CHP unit, releasing heat that is supplemented by burning the offgas from the HP and upgrading unit in a gas boiler. In the model, the CHP unit has an electrical efficiency of η_{el} = 0.39

Table 5
Utility demand and production.



	Heating [kW]	Cooling [kW]	Electricity [kW]	CHP power (W) [kW]	CHP heat (Q) [kW]	Q boiler (excess biogas) [kW]	Q boiler (offgas) [kW]
Scenario 1	376.99	-340.853048	30.74	30.74	40.98	22	63.18
Scenario 2	363.16	-336.88	29.75	29.75	39.66	160.58	52.37

and a thermal efficiency of $\eta_{\text{therma l}} = 0.52$. The gas burner has a thermal efficiency of $\eta_{\text{thermal}} = 0.98$.

For scenario 1, almost half of the remaining biogas is used for steam reforming to hydrogen, and 15.2 kg h^{-1} are sent to the CHP Unit to cover the plant's electricity demand of $W_{\text{plantutility}}$ = 30.7 kW (see Table 5). For the low-yield scenario 1, 4.3 kg h^{-1} excess biogas that could be fed to the natural gas grid is produced. For scenario 2, 25% of the biogas produced is used to supply hydrogen to the upgrading unit, and another 24% is sent to the CHP Unit to cover $W_{\text{plantutility}}$ = 30 kW. In scenario 2, excess biogas is available to be fed to the gas grid.

From Table 5, it is clear that the potential for heat integration and optimisation is high. A more detailed study of temperature levels, including pinch analysis, is necessary to determine how much of the cooling can be reused for heating, but the overall plant setup is well balanced.

Furthermore, this plant design offers possible solutions for and simplification of the issues of existing biogas plants. Because the digestate is directly converted after production in the biogas plant, no large storage tanks are necessary; the disposal problem discussed in Section 1 could be solved, and at the same time fertiliser could be extracted from the waste water. .Analysis of the waste water from the hydrothermal liquefaction processes has not been available other than with respect to the contents of fatty acids and alcohols (Toor et al., 2012). It is therefore important to investigate the fertiliser value of the waste water. Depending on the concentration of the nutrients like to nitrogen, phosphor and potassium it might be more cost-effective to either extract the nutrients and sell them as solids or pass on the waste water as an untreated liquid.

One method to increase the oil yield from the process would be to provide a digestate feed with a higher DM content to the HTL plant. This could be achieved, for example, by not converting the input manure fully in the biogas plant, but only converting the easily digestible part. The biogas yield would indeed be lowered, but as the production rate strongly decreased over time, the effect would likely be limited. However, a significant increase in high-value fuel yield would be expected from this. Other plant issues may arise from this method, especially regarding heat utility. Another method to increase the DM content would be to include a higher amount of bedding material, such as straw, in the input to the HTL plant in addition to high water-content manure and increasing the dry matter content to DM = 27–55 wt.% (Edström et al., 2011). Other streams of biomass could also be considered for increasing the DM content. To be able to supply more biomethane from biogas to the gas grid, other sustainable sources of hydrogen should be identified. Hydrogen could be produced by electrolysis using renewable electricity from wind or solar. This would help to reduce the impact of fluctuating sources of electricity on the electric grid. But also recycling the remaining hydrogen in the offgas stream from the HPU and upgrading unit instead of burning it in a gas boiler would higher the sustainability of the plant. Because all calculations are based on model components, it would be of great interest to further characterise biocrude from HTL and biofuel from upgrading in future studies and to develop a more precise model composition of biomass, biocrude and biofuel. Similarly, kinetic studies of the relevant reactions should be performed, which would make it possible to have yield-based simulation results and to perform a sensitivity analysis. Further work will include experimental studies on the liquefaction of different digestates and on the development of a heat recovery system for the overall plant design, which allows determination of economic feasibility of such a plant.

4. Conclusion

The prospect of biofuel production based on digestates from biogas plants is appealing. From low-energy–density manure with a LHV of 2.2–2.8 MJ kg^{-1} (Edström et al., 2011), a high-value diesel-quality fuel with a LHV of approximately 43.1 MJ kg^{-1} can be obtained. A 1000 kg h^{-1} substrate slurry input results in 36.8 kg h^{-1} biofuel for scenario 1 and 30.3 kg h^{-1} biofuel for scenario 2, which corresponds to 322.3×10^3 kg a^{-1} fuel and 265.4×10^3kg a^{-1}. The plant energy efficiencies are 62% and 84%, respectively, for the two scenarios, as calculated after accounting for the electricity demand of the plant.

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Paper 8

A simulation study of Solid Oxide fuel cell for IGCC power generation using Aspen Plus

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A simulation study of Solid oxide fuel cell (SOFC) for IGFC power generation using Aspen Plus

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Abstract The solid oxide fuel cell (SOFC) is a promising technology for electricity generation. Sulfur free syngas from the gas cleaning unit serves as a fuel for SOFC in IGFC (Integrated gasification Fuel cell) power plant. It converts the chemical energy of the fuel gas directly to electric energy and therefore, very high efficiencies can be achieved. The high operating temperature of the SOFC also provides excellent possibilities for cogeneration application. The outputs from SOFC can be utilized by HRSG which helps to drive steam generator. Recent developments in modeling techniques has resulted in a more accurate fuel cell model giving an advantage over previous system studies based on simplified SOFC models. The objective of this work is to develop a simulation model of a SOFC for IGFC system, flexible enough for use in future development, capable of predicting system performance under various operating conditions and using diverse fuels. The SOFC stack model developed using the chemical process flow sheet simulator Aspen Plus which is of equilibrium type and is based on Gibbs free energy minimization. The SOFC model performs heat and mass balances and considers the ohmic, activation and concentration losses for the voltage calculation and some graphical presentation of those losses by using MATLAB software. A various range of syngas properties has been used for the simulation which is gathered from different literatures. The results indicate there must be tread off efficiency and power with respect to a variety of SOFC inputs. SOFC stack operation on syn-gas is compared to operation on different coal properties and as expected there is a drop in performance, which is attributed to increased input fuel and air flow due to the lower quality of the fuel gas.

Keywords SOFC, simulation, IGFC, syngas.

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1. Introduction

Behavior of coal contaminants toward potentially very clean, highly efficient integrated power generating system is becoming increasingly important from both a system's performance and endurance, as well as an environmental point of view. IGFC is a combined power generation system combining IGCC and high- temperature fuel cells. The integrated gasification fuel cell (IGFC) system includes an advanced, catalytic, high -methane gasifier (29% in dry syngas) and syngas cleaning to achieve low sulfur levels in the fuel cell feed gas. The fuel cell system is more expensive than a combustion turbine but that expense is counterbalanced by the decrease in the unit cost of upstream equipment due to the higher IGFC system efficiency (1). A wide variety of coals can be used, allowing the effective use of coal: Low- grade coals with high moisture content and low calorific values, such as brown and sub bituminous coals, are difficult to use in conventional pulverized coal-fired power generation, but can be used as fuel for IGCC or IGFC power generation through the relatively easy gasification process (2). IGFC systems are promising for efficient and clean power generation from domestic resources, but most IGFC system analyses performed to-date have used non-dime -nsional SOFC models that do not resolve many intrinsic constraints of SOFC operation. A simplified cell-level SOFC model will provide many more insights into SOFC operation at reasonable computation expense. A finite volume model is a capable choice (3). A hybrid system of the solid oxide fuel cell (SOFC) with gas turbine has been studied for long times of period in the field of Energy conservation. A literature survey indicates that past research and development of SOFCs for large power systems has made significant advances since the early 1990s, research by Harvey and Richter (4). Fuel cell system control and design has received increasing attention throughout the years considering as well energetic and economic aspects and using sensitivity analyses (5). Afterwards, George (6) described a field unit demonstration program; including the Southern California Edison 220 kW pressurized SOFC/gas turbine (PSOFC/GT) power system, along with planned demonstrations of commercial prototype power systems from Siemens Westinghouse Power. As regards the heat exchangers and the heat recovery steam generator, all characterized by a tube-in-tube counter flow arrange ment, the simulation is carried out using the thermal efficiency-NTU approach (7). He also analyzed the Energy and exergy balances are performed not only for the whole plant but also for each component in order to evaluate the distribution of irreversibility and thermodynamic inefficiencies.

In this paper, a simulation model of a SOFC for IGFC system has been estimated and also the voltage calculation has been done. Considering the contribution of different components in the cycle, an algorithm has been then developed using ASPEN plus and MATLAB to simulate the performance of SOFC for IGFC cycle. This simulation will investigate the effects of various performance parameters, like SOFC fuel and air inlet temperature and flow rate.

2. SIMULATION MODEL

The stream 'SYNGAS' is fed to the 'COMPR1' block, simulating the fuel compressor. The discharge pressure was calculated by assuming a pressure ratio: P_{fuel}/P_{SOFC} = 3 (8). The syn-gas stream composition and thermodynamic condition were inputted; its mole flow rate is set by a design spec and depends on the specified stack power. The pressurized fuel is brought up to the fuel preheat temperature in the block 'FUELHEAT' and its exit stream enters the 'EJECTOR' block, where it is mixed with the recycled depleted fuel (stream 27). The pressure of the mixed stream (stream 4) is decreased back to slightly above atmospheric pressure (P_{SOFC}) and is directed to the 'COOLER' block. The two blocks 'COOLER' and 'PREFORM' simulate the operation of the pre-reformers. The purpose of 'COOLER' is to set the pre-reforming tempe-rature. It is calculated by means of a design spec, which varies the temperature of 'COOLER' until the net heat duty of 'PREFORM' equals zero (adiabatic). As a result, the gas is cooled simulating the endoth-ermicity of the steam reforming process. The following chemical reac-tions were specified in the 'PREFORM' block:

Steam reforming : $CH_4 + H_2O = 3H_2 + CO$ (1)

Water-gas shift : $CO + H_2O = CO_2 + H_2$ (2)

It was assumed that the reactions reach thermodynamic equilibrium at the pre-reforming temperature. The pre-reformed fuel (stream 6) is fed to the 'ANODE' block, where the remaining CH_4 is reformed, CO is shifted and H_2 is oxidized. In a SOFC the following reactions occur:

Cathode half reaction : $0.5O_2 + 2e^- \rightarrow O^{2-}$ (3)

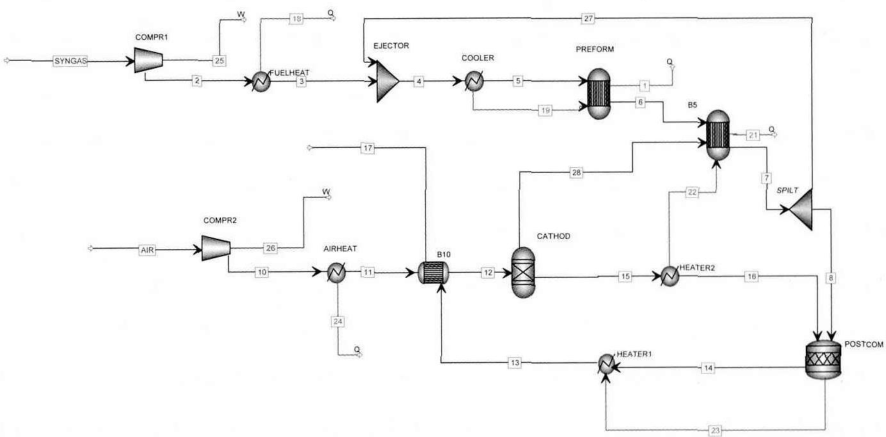
Anode half reaction : $H_2 + O_2 \rightarrow H_2O + 2e^-$ (4)

Overall reaction : $H_2 + 0.5O_2 \rightarrow H_2O$ (5)

The oxygen ion O_{2-} is the charge carrier in a SOFC. It is transported through the electrolyte to the anode side where it reacts with H_2 to produce electrons e−. The transfer of ions cannot be modeled in Aspen Plus; therefore the overall reaction instead of the cell half reactions was used in the simulation. Although it is possible to directly oxidize CH_4 and CO in a SOFC at its high operating temperature, it is common to assume that the CH_4 is reformed and the CO is shifted to H_2 and therefore only H_2 participates in the electrochemical reaction. Reactions (1), (2) and (5) were specified in the 'ANODE' block and it was assumed that they reach thermodynamic equilibrium at the block temperature the oxidant (stream 'AIR') is fed to the 'COMPR2' block, the air com-pressor. Its discharge pressure was set as slightly above atmospheric pressure (P_{SOFC}). The air stream composition and thermodynamic condi tion were inputted. The molar flow rate is determined using a design spec that varies the air flow until the air utilization factor U_a = 18% (9). The compressed air is brought up to the air preheat temperature in the block 'AIRHEAT' and its exit stream enter 'B10' where it is preheated further by the hot combustion plenum products. The com ressed and preheated air (stream 12) enters the 'CATHODE' block, whose function is to separate out the O_2 required for the electrochemical reaction.

The temperature of the depleted air (stream 15) must be increased to the stack operating temperature (*Top*). The heat needed to do this is supplied by the electrochemical reaction and this process was simulated by taking a heat stream (22) from 'HEATER2' to 'ANODE' . The tempera-ture of the 'HEATER2' block was specified. The depleted fuel (stream 7) enters the block 'SPLIT' , whose function is to split the stream into a recycle (stream 8) and a stream directed to the combustion plenum. The split fraction of the block is set using a design spec where it is defined as the molar ratio of steam to combustible carbon, a typical value being 2.5. Excess steam as well as increasing the concentration of H_2 and CO_2 inhibits the formation of carbon. Carbon deposition not only represents a loss in the system but results in deactivation of catalysts and decreases the activity of the anode by clogging the active sites. The depleted fuel and oxidant are fed to 'POSTCOM' where complete combustion of the remaining fuel occurs. The following combustion reactions, assumed to reach completion, were specified:

[Figure 1] Aspen Plus flow sheet of the SOFC stack.



$$H_2 \text{ combustion : } H_2+0.5O_2 \rightarrow H_2O \quad (6)$$

$$CO \text{ combustion : } CO+0.5O_2 \rightarrow CO_2 \quad (7)$$

$$CH_4 \text{ combustion : } CH_4+O_2=2H_2O+CO_2 \quad (8)$$

The heat generated by the reactions is calculated and is put into the heat stream 23, which is fed to the block 'HEATER1', whose function is to calculate and set the combustion products temperature. Finally, the high temperature combustion products (stream 11) exchange heat with and serve to preheat the incoming air in the 'HEATX1' block. The temperature of the SOFC stack exhaust (stream 12), which may be utilized in a district heating system, is also determined.

3. RESULTS

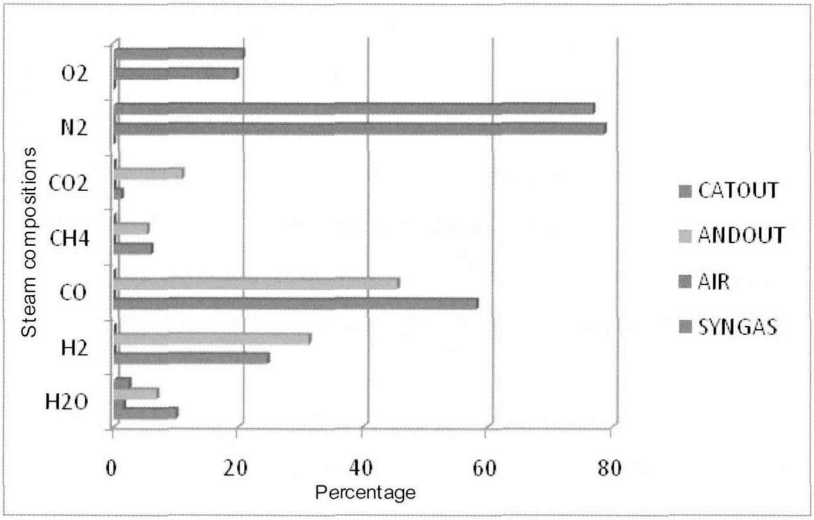
The SOFC inlet and outlet temperatures for this analysis were assumed to be 750℃ and 815℃, respectively. The electrolyte of a SOFC operates between 600 - 1000℃ where ionic conduction by oxygen ions takes place.

In simulation A fuel flow is 80000 (kg/hr) and air flow rate is 68038 (kg/hr). As the SOFC simulation is considered as pressurized model so ejector pressure ratio has selected as 3 and 4 for the simulation "A" and "B" respectively.

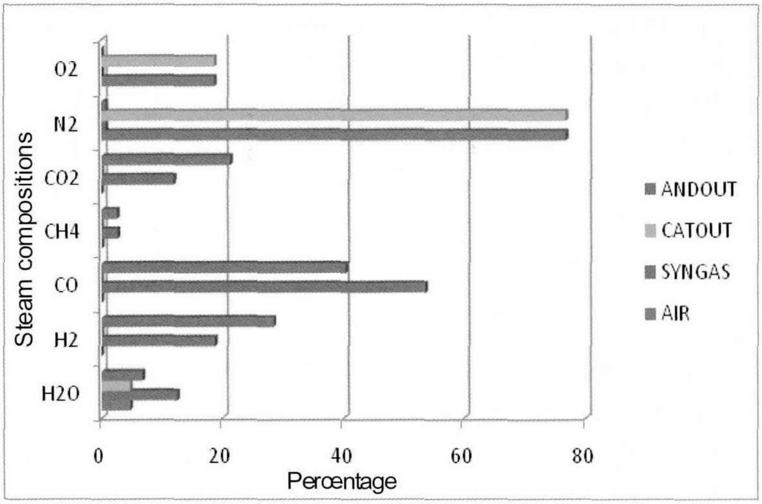
From the two simulation, simulation A has selected as it was more familiar with the literature. Here just show the data for steam Anode out and the cathode out for simulation A. Fig.2 and Fig.3 show that the variation of mole percentage in syngas input, air inlet and Anode, cathode outlet for simulation 'A' and 'B' respectively.

The fuel cell operating parameters used to develop this case are shown in Table 5. The voltage loss for the different earlier mentioned losses is almost 5 percent of the total voltage. And the current density consider for this case is 1800 mA/cm^2. Fuel utilization is 75% for this case where air utilization is 18%.

[Figure 2] Percentage of different components for simulation 'A'.



[Figure 3] Percentage of different components for simulation 'A' and 'B'.



[Table 1] Fuel Cell Operating Parameters.

Parameter	Value
Nernst Potential, V	0.76
Operating Voltage, V	0.72
Fuel Utilization %	75
Air Utilization %	18
Current Density, mA/cm^2	1800
Anode Gas Recycle, %	30

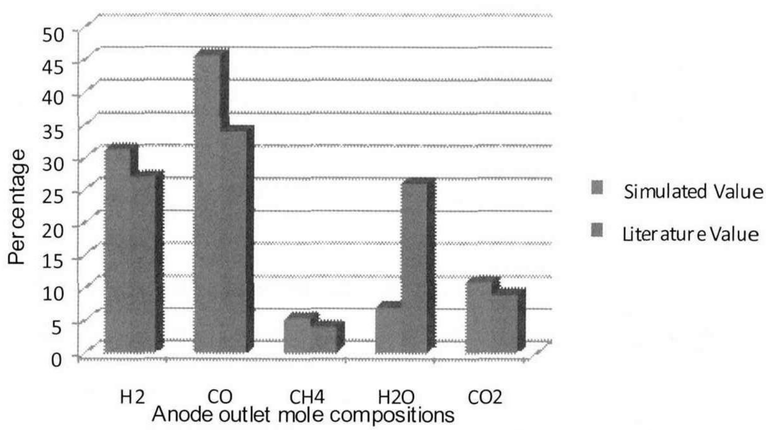
4. Model validation

The developed model was validated against published data for the NETL 300 MW IGFC combine cycle SOFC stack operating on coal [10]. Table 11 shows the comparison between the simulated value and the literature value for the SOFC part. Operating pressure is higher than the literature value and the reforming percentage is 30 which may effects on fuel utilization factor. SOFC efficiency is measured by the Eqn. (16-19) using simulation results. It can convert 95% of DC current to AC current

[Table 2] Data for model calibration.

Parameters	Simulation	Literature
Single Cell Voltage, volts	0.72	0.69
Current Density, A/m^2	1800	-
Operating Pressure, psia	19.5	18
Air Intake rate, Ib/hr	68038	78500.6
Pre-reforming Percentage, %	23.6	-
Compressor Pressure Ratio	3	-
Fuel mass flow ,Ib/hr	80000	96514
Cathode exhaust gas Composition (mole %)	N_2=76.9, O_2 =18.56, H_2O=4.18, H_2=0.36	N_2=80, O_2= 18, H_2O=2
Fuel utilizationa (%)	72	-
Air utilization (%)	18	-
System Fuel Effectiveness with IGFC, %	86.6	-
Inverter efficiency (%)	95	92
Gross AC efficiency (LHV) (%)	52	51.5
SOFC efficiency (%)	59	

[Figure 4] Comparison of Anode outlet composition



From the two simulation, simulation A has selected as it was more familiar with the literature. Table 3 shows the some output parameters of the Aspen Plus simulation. Here just show the data for steam

Anode out and the cathode out for simulation A. As in this model water circulation has not involved so the percentage of H_2O in the anode outlet gas composition is lower than the literature data (Fig.4).

The model results are primarily constituted by the total cell balances and by total cell internal profiles for any relevant thermodynamic or electrochemical variables. The comparison results documented in Table 2 confirm that the system can be improved by operating the SOFC at temperature, pressure, and flow rates and so on. The exhaust gas from the anode will utilize by HRSG for producing hot steam for the steam turbine.

5. CONCLUSION

In the IGFC configuration, power is generated by both the fuel cell and the steam cycle. The fuel cell is the most efficient energy conversion device in the cycle. Therefore, system efficiency should improve as energy conversion in the SOFC is optimized, in terms of fuel utilization and overpotential reduction. In this study fuel cell efficiency is measured.

A simulation model of the SOFC stack was developed using Aspen Plus. The main purpose of this work was to develop a computer simulation model flexible enough for use in future study and industrial uses and capable of predicting system performance under various operating conditions and using different coal for variation in syngas properties, was achieved. Two methods have done for SOFC simulation and select simulation 'A' for the further simulation as it has better output results for HRSG operation.

A sensitivity analysis applied to the model parameters has shown the effect of different hypothesis for the evaluation of the cell losses, as well as of the cell internal heat exchange processes and of hydrocarbons reforming reactions. Among other results, it is shown that the importance of the adoption of appropriate parameters for the evaluation of activation polarization, as well as the relevance of a kinetic model for reforming reactions.

Finally, the results of the cases presented in the result section illustrate how an IGFC system has more efficiency benefits over other advanced power generation technologies. If advanced fossil energy research goals in the areas of coal gasification and solid oxide fuel cell development are met, this study demonstrates an IGFC combined cycle of 48.28 % efficiency.

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