

# Energy integration and analysis of SOFC based micro-CHP and other renewable systems using biomass waste derived syngas

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## Abstract

The objective of this paper was to design energy integrated solid oxide fuel cell (SOFC) based micro-combined heat and power (micro-CHP) systems using syngas derived from lignocellulosic biomass waste. The novel contributions of this work include 1) integration of syngas between a community-scale biomass gasification plant and SOFC based micro-CHP systems in buildings; 2) heat integrated designs of SOFC based micro-CHP systems; 3) integration between SOFC and other heat-led renewable technologies, such as, syngas boilers, ground source heat pump (GSHP) and air source heat pump (ASHP). Conceptual process design frameworks including detailed heat recovery strategies were developed using Aspen plus. It is demonstrated that increases in heat integration between the SOFC inlet and outlet gases enhance the power-to-heat generation ratio from the SOFC albeit at a higher cost of heat exchanger area. A straw (14.6 MJ/kg LHV) based community-scale gasification plant can generate 50-100 kW<sub>e</sub> of electricity at an overall CHP generation efficiency of ~42%, while if integrated to SOFC based micro-CHP systems (1 kW<sub>e</sub>) in individual dwellings via syngas, the overall energy efficiency can be greatly enhanced to ~85%. It is envisaged that the SOFC should be operated at the highest electrical efficiency based on optimal heat integration, however, this needs to be coupled to other heat-led renewable technologies in order to meet the high residential heat to power demand ratio in the UK. Around 2.2 times more syngas may be required in boilers for supplementing residential heating. In integration with a GSHP loop, the flue gas from SOFC can itself be used as a refrigerant and energy integration between the two systems can achieve an overall efficiency of ~90%.

*Keywords:* distributed energy, syngas to micro-CHP, residential energy, fuel cell, ground source heat pump and SOFC integration, biomass waste gasification

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## 1. Introduction

The concept of microgeneration implies to combined heat and power (CHP) generation with low or zero carbon emission, by individuals, businesses and communities, at or near the point of use<sup>1-2</sup>. The UK Government made an important commitment in the Energy Act 2004 by developing an ongoing microgeneration strategy in order to create a sustainable residential energy market and thereby tackle its contribution to climate change<sup>2-3</sup>. The microgeneration or self generation concept for dwellings is associated with several advantages, such as follows:

- (1) Cutting emissions of greenhouse gases
- (2) Reducing the number of people living in fuel poverty
- (3) Reducing the demands on transmission systems and distribution systems
- (4) Reducing the need for those systems to be modified
- (5) Enhancing the availability of electricity and heat for consumers
- (6) Encourage consumer engagement with energy efficient technologies

The micro-CHP in this paper is referred to the generation of 1 kW<sub>e</sub> of electricity from a dwelling installation<sup>1-4</sup>. This is differentiated from a community-scale (multi-dwelling) electricity generation in the range of 50-100 kW<sub>e</sub><sup>4</sup>. The community generation is referred to the supply of heat or combined heat and power from a central source to a set of buildings in a community. It also allows customers from various sectors such as domestic, schools, offices, as well as industrial sectors. As identified in many studies by the Energy Saving Trust, the main potential use of micro-CHP is in conjunction with community based generation schemes<sup>1</sup>.

Fuel cells have become a very important energy technology in the UK and worldwide, due to their inherently clean, greener and efficient operation. The SOFC can be used to micro generate electricity and

heat simultaneously and have therefore become very relevant for dwelling micro-CHP generation. The SOFC can utilise heat of oxidization of gaseous fuels such as hydrogen, syngas, natural gas, etc. in the anode in the presence of an oxidant in the cathode, into electricity. The performance of a SOFC when fuelled directly with pure hydrocarbons, such as, methanol, has also been investigated and for the application in electric vehicles<sup>5-7</sup>. Even greater environmental benefits can be gained if gaseous fuels, such as syngas from waste materials, which is a good source of renewable hydrogen, can be used as a fuel to the SOFC<sup>8-9</sup>. Our previous study included performance analysis of overall integrated biomass gasification fuel cell systems in one infrastructure, in which the exhaust gases from a SOFC were fed to an interconnected fluidized bed biomass gasifier, in addition to the integration of the syngas from the gasifier to the SOFC<sup>9</sup>. Such schemes exploiting high temperature heat and material integration between the gasifiers and SOFCs can be implemented for community scale generations. More recently, the SOFC has also been studied for application in residential micro-CHP<sup>10-14</sup>. Authors have investigated into the viability of newly developed micro-CHP concepts, e.g. fuel cells and sterling engines, integrated with thermal storage units, etc. in the context of UK's residential heat and power demands, economics and energy policies.

The UK renewable energy roadmap shows solar heat, biomass boilers, ground source heat pump (GSHP) and air source heat pump (ASHP) as the main heat-led technologies<sup>15</sup>. Typically, 68-82% (new – existing buildings respectively) of the residential energy is required in the form of heat, such as residential hot water and space heating<sup>10-14</sup>. A micro-CHP system in the UK thus generally invokes heat-led renewable technologies alongside with connection to national electricity grid in order to ensure a consistent supply of power. The heat-led micro-CHP has less consistency in operation in summer months when there is little or no heat demand. The SOFC can substitute heat-led micro-CHP and enable onsite power generation renewably and effectively. The SOFC have high electrical efficiency and low heat-to-power ratio. Thus, if applied to a single household in the UK, the thermal efficiency, hence CHP generation efficiency needs to be enhanced significantly, without compromising on the electrical efficiency. The objective of this study

was the heat integrated design of high efficiency SOFC for UK residential micro-CHP. Heat recovery from the exhaust gas from SOFC operating at elevated temperatures of above 500°C, can significantly enhance the overall CHP generation efficiency. Additionally, thermal coupling between SOFCs and heat storage systems can be considered to respond to large rapid residential heat demands<sup>13</sup>. This work further investigates into the integration of SOFCs with other forms of heat-led renewable technologies, such as the GSHP and ASHP systems, identified for UK micro-CHP applications<sup>15</sup>, using conceptual low temperature heat integration approaches<sup>16-17</sup>. The SOFC, an effective power-led technology, and GSHP that utilizes ground-based energy into useful heat generation, are complementary to each other. There exists a good thermodynamic integration synergy between them, which must be explored using theoretical and conceptual studies before any expensive demonstration work, in order to comprehend the basic structure, efficiencies and directions for further research<sup>15</sup>, which is the objective of this study.

The modeling of fuel cells spans from electrochemical reaction and mass and heat transport modeling<sup>18-20</sup> to detailed microstructural modeling<sup>21</sup> and multi-scale modeling, e.g. CFD<sup>22</sup>, approaches. Detailed modeling of SOFC is not within the scope of this study. For the conceptual heat integrated designs of SOFC, an Aspen Plus<sup>23</sup> simulation framework for the generation of kinetic parameters and mass and energy balances<sup>9</sup> and an Excel based irreversible steady-state model, wherein irreversibilities resulting from electrochemical reaction, electrical resistance, and heat transfer to the environment were taken into account<sup>18-20</sup>, were used. This paper is structured as follows. The first section has highlighted the main features of the straw based community-scale gasification plant under consideration<sup>24</sup>. Provisions to generate clean syngas fuel from the biomass gasification plant for SOFC based micro-CHP systems as well as CHP using gas turbine based combined cycle were considered. Thereafter, the heat integrated high efficiency SOFC schemes that utilise straw derived syngas have been presented. Finally, integration between SOFC based micro-CHP schemes and supplementary firing, and GSHP and ASHP systems is analysed in response to high energy demands by the UK residential sector. Each section contains an Aspen Plus simulation based energy integration methodology and analysis of results for respective systems.

## 2. Design of biomass waste based small scale community-scale generation of syngas and CHP

The SOFC based micro-CHP designs analysed were based upon syngas as the feedstock derived from agricultural wastes, such as straws. The gasification technologies can be used to thermo-chemically convert biomass (waste) into energy products, such as syngas. Gas is the most common fuel for building energy supply<sup>1</sup>. An equivalent replacement of the gas is biomass-based syngas, which can be used in individual micro-CHP installations in buildings. Additionally, a combined cycle gas turbine utilizing syngas can also be applied to the community-scale biomass gasification plant, in order to generate CHP in large scale, discussed in this section. This is to meet the peak power and heat demands by community dwellings or any other customers and to sell back any excess electricity and heat to the national grid. Fig. 1 illustrates the integration synergy between a large scale biomass gasification plant and SOFC based micro-CHP systems in buildings via syngas.

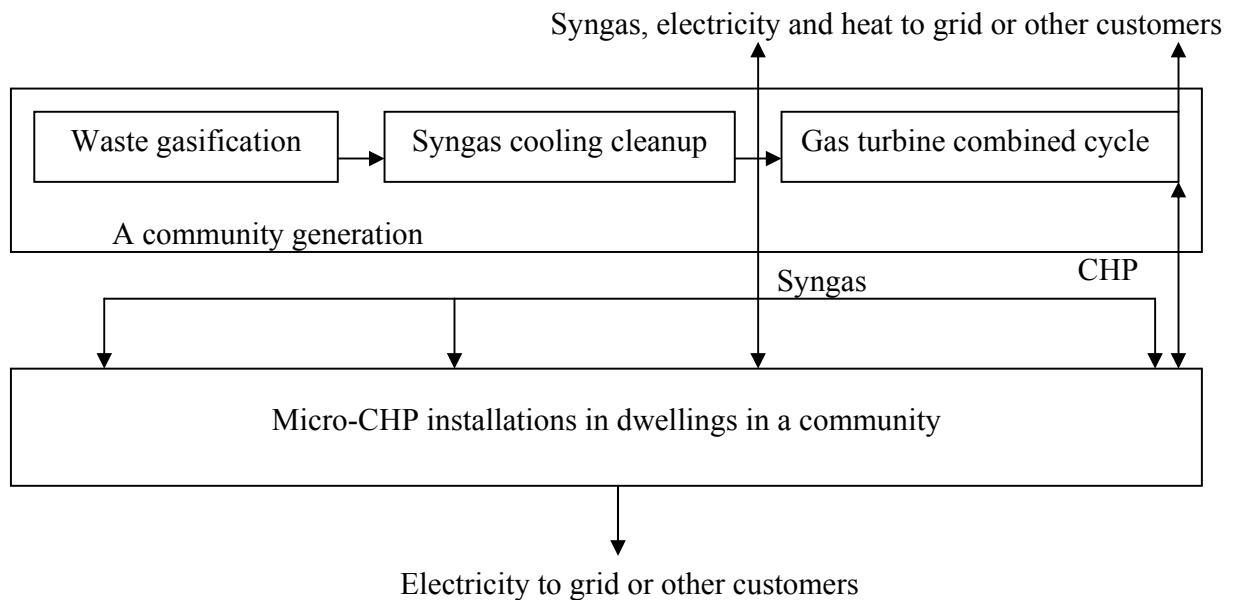


Fig. 1. Integration between community-scale biomass-based syngas and CHP plant and SOFC based micro-CHP systems in buildings.

The biomass gasification plant under consideration comprises gasifiers, gas cooling and clean up technologies, gas turbines and heat recovery steam generators (HRSG), etc. The first three unit operations are used to produce clean syngas feedstock for SOFC and / or gas turbine combined cycle, while the latter two operations are investigated for CHP generation. The integration strategies developed for community-scale syngas and CHP generation plant based on agricultural wastes, straws<sup>25</sup>, in view to improve energy efficiency, heat recovery and cleaner operations, are as follows. The performance of the biomass gasification plant was validated against literature<sup>25-27</sup> and the results are presented elsewhere<sup>24</sup>.

The gasification process under consideration comprises two interconnected pressurized and high temperature fluidised bed reactors: air blown char combustor for the unreacted char (also ash) and steam gasifier for the rest of the biomass, gas and tar<sup>25-27</sup>. The flue gas from the air blown char combustor (containing nitrogen and carbon dioxide as the main constituents) and the product gas from the steam gasification (containing hydrogen and carbon monoxide as the main constituents) can be added together, resulting in a product syngas with an appropriate level of hydrogen concentration. An adequate level of hydrogen concentration, heating value and lower temperature (than the gasification) of the clean syngas product makes it a good transportable feedstock to the SOFC based micro-CHP systems as well as for combustion in gas turbines onsite. Furthermore, the lower inlet temperature of the syngas feed controls the temperature rise in the gas turbine combustor. Consequently, the requirements for dilution with inert gas in order to lower the NO<sub>x</sub> emission from the gas turbines are minimised. The resulting syngas produced from the air driven steam gasification process after high temperature cleaning and cooling can directly be quenched with cooling water below its dew point (~60°C) so as to allow the separation of water and tar condensables, leaving the gas clean and dry and improving its heating value. This maximizes the heat recovery from the high temperature syngas from the gasifier and minimizes the heat loss during gas clean-up. The effluent water recovered from syngas cooling below its dew point, after purge and waste water treatment can be recycled to the syngas cooler for high pressure superheated steam generation. The balance of the steam generation from HRSG and syngas cooler and the steam consumption by the steam

gasification unit and other cleaning processes, such as, the Rectisol process, developed by Lurgi and Linde<sup>28</sup>, can be made available as residential heat, which can enhance the overall energetic efficiency of a biomass gasification combined cycle plant. The Rectisol technology provides an excellent option for co-removal of a number of contaminants to a trace level (for e.g. H<sub>2</sub>S to less than 0.1 ppm by volume), using one integrated plant. A syngas feed to SOFC needs to be cleaned at 0.1 ppm level of purity of H<sub>2</sub>S<sup>8</sup>. The syngas capacity reported is in the range of ~100-350 Nm<sup>3</sup>/hr<sup>28</sup>, which is in this case 337 Nm<sup>3</sup>/hr.

The straw based gasification process flowsheet with the provisions to produce the clean syngas fuel to the SOFC based micro-CHP systems as well as CHP from gas turbine – HRSG based combined cycles was simulated in AspenPlus. The Non-Random Two Liquid (NRTL) thermodynamic package was used for the estimation of physical properties. The operational specifications of these processes for the delivery of a cleaner form of syngas and CHP in Aspen simulation are presented in Table 1. The biomass (without the ash) compositional analysis has been entered as gas, tar and char provided in Table 2<sup>26</sup>. These are the primary pyrolysis derived from a biomass. A biomass devolatilises into gas (comprising of hydrogen, methane, C<sub>2</sub>: ethane and ethylene, carbon monoxide, carbon dioxide and steam) and tar, leaving behind solid char, as soon as it comes in contact with the hot bed of a gasifier and before any mixing / mass transfer for gasification reactions takes place, thus it's practical to deal with the gas, tar, char and ash components separately in a simulation model<sup>26, 29</sup>. Tar was modeled as phenol as revealed in numerous studies<sup>26, 30</sup> and as steam and oxygen to balance the C, H and O contents in the biomass (Table 1). Biomass char and ash were modeled as non-conventional components. The interconnected circulating fluidised bed gasifier in Aspen simulation in Fig. 2 consisted of two RGibbs reaction modules: steam gasification of gas and tar and combustion of char with air. Ash has been removed as an inert from the bottom of the char combustor, followed by its removal from a hot gas filtration. The RGibbs reactor of Aspen that works on the Gibbs free energy minimization principle has been widely adopted to represent gasification reactions<sup>24-26</sup>.

Table 1. Aspen modelling and operating conditions for various processes in biomass gasification based CHP flowsheet and SOFC based micro-CHP systems

Process	Aspen model used	Specifications		
		Temperature °C	Pressure bar	Any other conditions
Gasifier	Gibbs reactor for steam gasifier and char combustor	>900	7-10	
Steam to gasification		<750	7-10	Steam to biomass ratio: 0.6
Gas after primary pyrolysis	Modeled as in Table 2	>900	7-10	
Tar after primary pyrolysis (molar concentration)	Phenol: 0.46 Steam: 0.21 Oxygen: 0.33	>900	7-10	
Char after primary pyrolysis	Carbon (Table 2)	>900	7-10	
Air (molar concentration)	Oxygen: 0.21 Nitrogen: 0.79	20	1.013	
Stoichiometric oxygen				To char combustor: 21.9 kg/hr To GT combustor: 925.8 kg/hr
Air compressors	Compressor		7 (exit)	Efficiency: 0.9
Syngas cooler	Cooler	60 (exit)	7	
Effluent recovery / Direct quench	Flash separator	50	7	
Steam to combined H <sub>2</sub> S and CO <sub>2</sub> recovery		150	3	H <sub>2</sub> S recovery: 99% CO <sub>2</sub> recovery: 90%
GT combustor	Conversion reactor 90% conversion	900	7	Feed gas Wobbe Index: 9-11
Expanders	Expander		1.05 (exit)	Efficiency: 0.9
HRSG	Cooler	50 (exit)	1.013 (exit)	
SOFC preheaters	Heat exchangers	Table 6	1	
SOFC cathode	Separator	800	1	
SOFC anode	Gibbs reactor	800	1	
SOFC exhaust condenser	Heat exchanger and Flash separator	60 (exit) 58 (exit)	1 1	



Table 2. Composition of biomass (gas, tar and char) after primary pyrolysis or devolatilisation<sup>26</sup>

Component	kg/kg biomass
Total gas	0.48
H <sub>2</sub>	0.00
CH <sub>4</sub>	0.02
C <sub>2</sub>	0.12
CO	0.22
CO <sub>2</sub>	0.03
H <sub>2</sub> O	0.08
tar	0.48
char	0.04

The Aspen based simulation framework for the biomass gasification plant in Fig. 2 also includes syngas coolers and heat recovery steam generators (HRSG) (modeled as coolers) as the main sources of high grade heat, effluent recovery unit (modeled as flash separators) as a source of low grade heat and water, air compressors and gas turbine expander as power consumption and generation units respectively. From the energy balance across the site, the net power obtained from the gas turbines after consumption in air compressors, is 61 kW<sub>e</sub>, assuming that all the excess heat generated from the site would be utilised in residential heating. Alternatively, the power to heat generation ratio can be enhanced by expanding steam through back pressure turbines, albeit at a lower efficiency of steam turbines. The results of mass and energy balances including the emission burdens of the biomass gasification plant for different energy supply scenarios from Aspen simulation are presented in Fig. 2. Fig. 2 demonstrates that based on a utilization of the maximum amount of syngas of 327 kg/hr, produced from gasification of a straw slurry flowrate of 227 kg/hr (14.6 MJ/kg LHV), an overall CHP generation efficiency of 42% can be obtained from the community-scale biomass gasification combined cycle plant. The contribution of heat (326 kW<sub>th</sub>) is about 85% of the total CHP generation including the low grade heat recovered from the effluent recovery unit (50.27 kW<sub>th</sub>), based on the scheme proposed in Fig. 2.

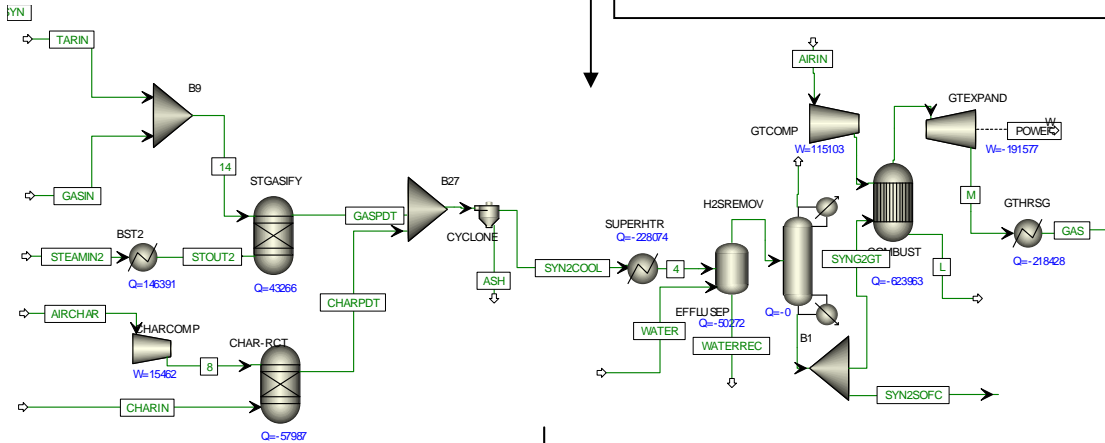
Biomass analysis<sup>25</sup> (227 kg/hr)

Straws

Proximate analysis (wt%)		Ultimate analysis (wt%)	
moisture	8.50	C	36.57
volatile matter	64.98	H	4.91
fixed C	17.91	O	40.70
ash	8.61	N	0.57
LHV	14.60 MJ/kg	S	0.14

Air (at 25°C, 1 bar pressure and 939 kg/hr; N<sub>2</sub>:O<sub>2</sub> mol ratio = 0.79:0.21)

Boiler feed water (at 25°C, 1 bar pressure and minimum flowrate 29 kg/hr)



Exhaust gas mol fraction (at 40°C, 1 bar and 1162 kg/hr)	Sulphur 0.248 kg/hr Ash 19.5 kg/hr	Syngas mol fraction (at 60°C and 5 bar pressure)*
H <sub>2</sub> O 0.199	Effluent water at 40°C, 1 bar and 12 g/hr	H <sub>2</sub> O 0.006
N <sub>2</sub> 0.637	*Based on a maximum of 327 kg/hr of syngas produced from biomass gasification 326 kW <sub>th</sub> and 61 kW <sub>e</sub> of heat and power can be generated.	N <sub>2</sub> 0.171
O <sub>2</sub> 0		O <sub>2</sub> 2.205e-05
NO <sub>2</sub> 0		NO <sub>2</sub> 0
NO 5.214e-07		NO 1.218e-06
S 0		S 0
SO <sub>2</sub> 6.389e-11		SO <sub>2</sub> 0
SO <sub>3</sub> 0		SO <sub>3</sub> 0
H <sub>2</sub> 5.958e-06		H <sub>2</sub> 0.440
CL <sub>2</sub> 0		Cl <sub>2</sub> 0
HCL 0		HCL 0
C 0		C 0
CO 6.220e-06	*Syngas < 327 kg/hr can be exported to micro-CHP systems and CHP generation from gas turbine combined cycle will be proportionally reduced.	CO 0.222
CO <sub>2</sub> 0.164		CO <sub>2</sub> 0.151
H <sub>2</sub> S 1.963e-08		H <sub>2</sub> S 4.583e-08
CH <sub>4</sub> 0		CH <sub>4</sub> 0.009
COS 3.954e-08		COS 9.231e-08

Fig. 2. Results of Aspen simulation of biomass gasification based CHP flowsheet (power (W) and heat (Q) generation / consumption are in Watt); SYN2SOFC is the syngas to be exported to SOFC based micro-CHP systems.

### 3. Design of SOFC based micro-CHP systems

A micro-CHP system for a single dwelling is desired to produce  $1 \text{ kW}_e$  of electricity<sup>1, 4</sup> and  $4\text{-}8 \text{ kW}_{th}$  of heat<sup>1</sup>. Syngas as a source of renewable hydrogen from the community-scale biomass waste based gasification plant illustrated in section 2 can be utilised in SOFC for the generation of power. A systematic heat integration strategy was developed to preheat SOFC feed gases to a maximum extent in order to enhance the total energy output from it, as depicted in Fig. 3 and discussed as follows. Preheating of syngas and air to SOFC can be achieved by exchanging heat with the outlet gases from SOFC, flue gas and nitrogen rich depleted air (with trace amount of oxygen) from anode and cathode, respectively, based on closer specific heat values between hot and cold streams (or uniform driving force across a heat exchanger). Preheating of feed gases facilitates endothermic reforming reactions and increases the net exothermic heat generation (due to combustion) from the SOFC. Since the Gibbs free energy change of an electrochemical reaction is a measure of the maximum electrical energy obtainable as work from the reaction, preheating of feed gases to a maximum feasible temperature (allowing  $20^\circ\text{C}$  minimum temperature approach between the hot and cold streams) ensures maximum energy output, hence, maximum power generation from SOFC (Option 1 in Fig. 3). However, the maximum preheating / power generation strategy is associated with the requirements of the maximum heat exchanger areas. Henceforth, a co-current preheating option was also explored, which maintains a tradeoff between power to heat ratio obtainable from the SOFC and the heat exchanger area required (Option 2).

In Option 1, after maximum preheating, the flue gas from SOFC anode still has residual low grade heat available, which can be recovered into cooling water, heated up to  $70^\circ\text{C}$  (as a source of residential heat). In Option 2, both the nitrogen rich depleted air from SOFC cathode and the flue gas from SOFC anode

after preheating would still be at a high temperature, hence they can be mixed together before heat recovery into cooling water for residential heating.

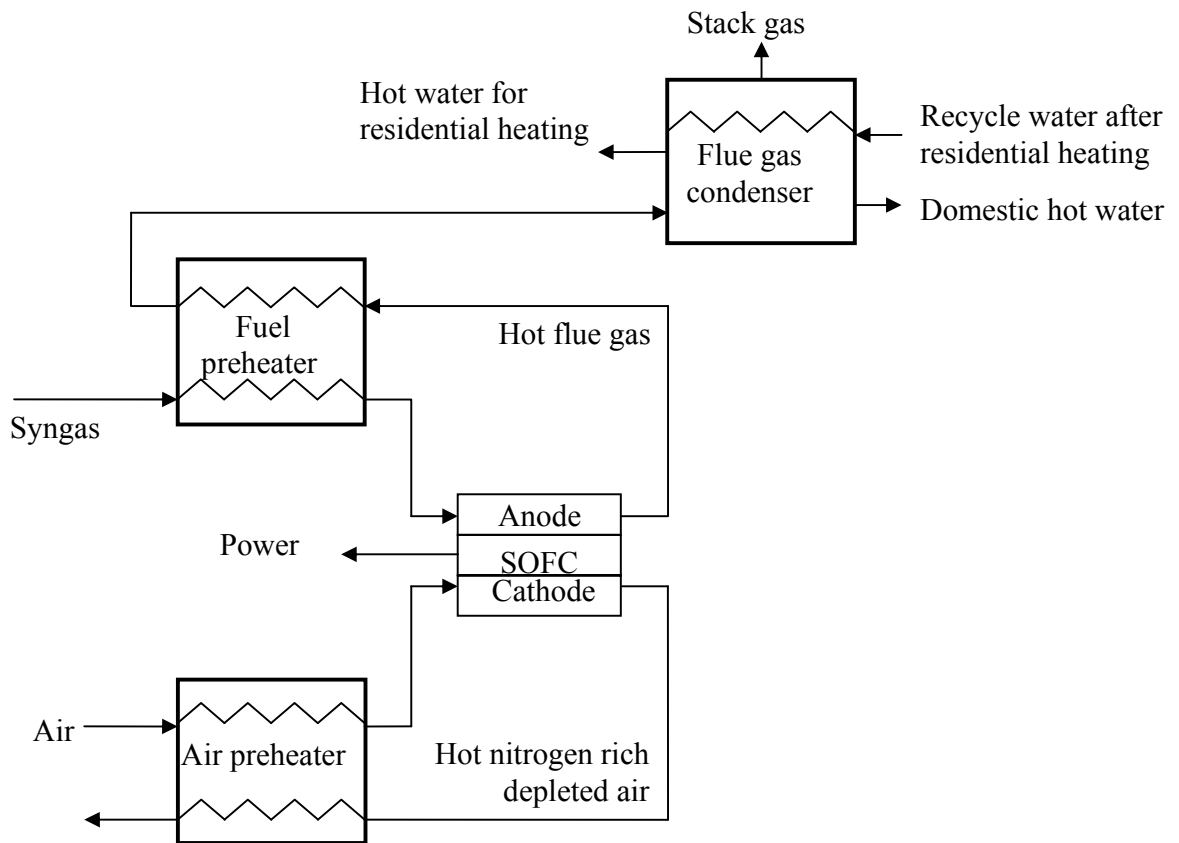
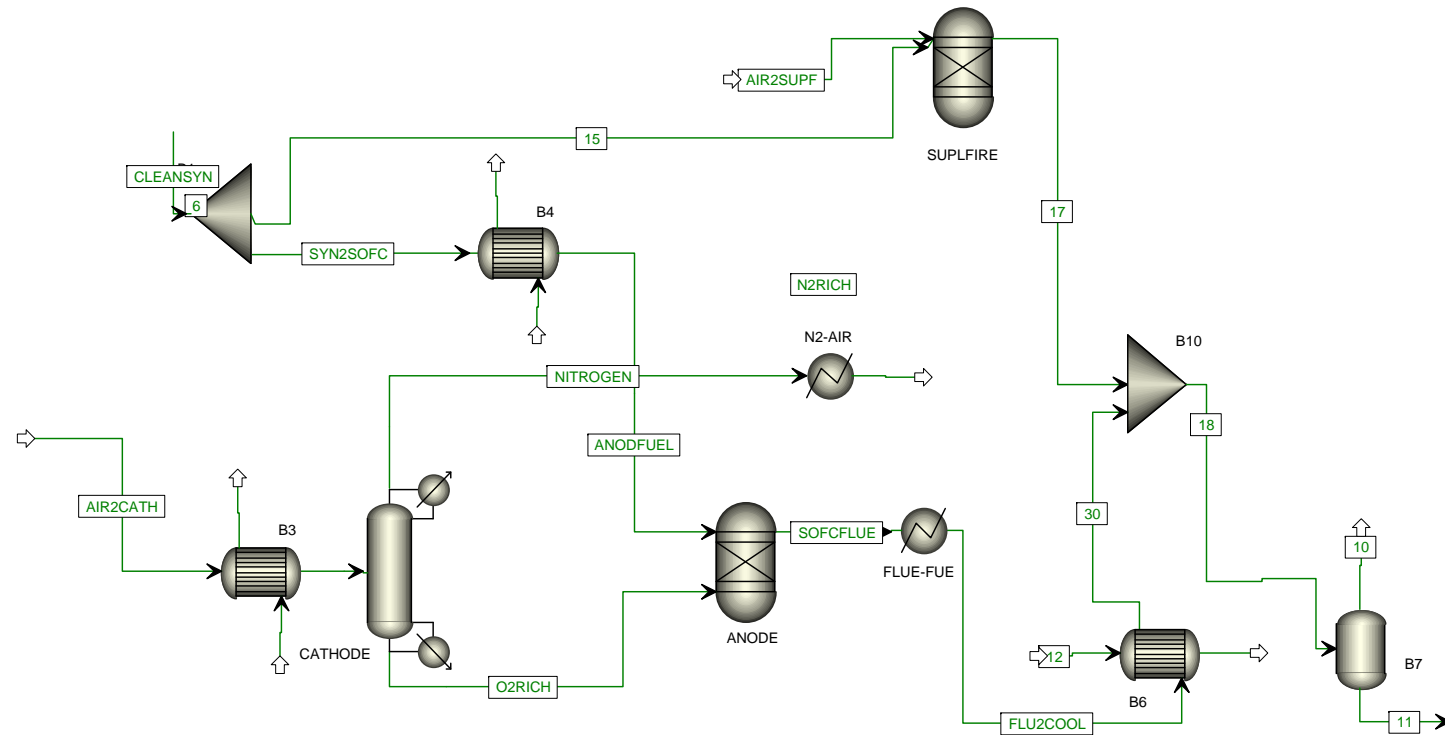


Fig. 3. SOFC scheme with counter-current preheating of air and syngas to SOFC by nitrogen rich depleted air and flue gas from SOFC respectively (Option 1).

In both the SOFC schemes, condensation of the exhaust gas below its dew point has been considered for low grade heat recovery. The resulting flue gas from the anode contains water and carbon dioxide as the main constituents in Option 1. In Option 2 the nitrogen rich depleted air and the flue gas from the SOFC are mixed and the mixed stream contains water, nitrogen and carbon dioxide as the main constituents. Hence condensation of the (mixed) flue gas below its dew point by cooling water results into a gas free water phase and a dry gas phase. Cooling water after recovering heat from the SOFC (mixed) flue gas to  $\sim 60^{\circ}\text{C}$  is circulated through buildings for residential space heating and returned back to the (mixed) flue

gas condenser (Fig. 3). The water phase recovered from the SOFC flue gas (at the dew point  $\sim 58^{\circ}\text{C}$ ) can be used as domestic hot water. Thus, a pure form of hot water generating from hydrogen in the SOFC feed gas can also be utilized into residential heating. The remaining dry stack gas may be exhausted into the atmosphere.

The basic working principle of SOFC is presented elsewhere<sup>18-20</sup>. Modeling of SOFC systems has two parts, simulation and heat integration in Aspen Plus and electrochemical modeling to predict the power output from SOFC. The various chemical reaction kinetic parameters obtained from an Aspen simulation were used in electrochemical modeling of SOFC to predict its output power generation. The modules in the SOFC system were simulated and heat integrated in AspenPlus in order to establish mass and energy balances (Fig. 4). The various process models and variables used are listed in Table 1. The SOFC cathode and anode were modeled as a separator and Gibbs reactor, respectively<sup>8-9</sup>. The oxygen rich gas is separated from the remaining nitrogen rich depleted air stream from the cathode and routed to anode, where oxidation of the syngas takes place producing the flue gas from the anode.

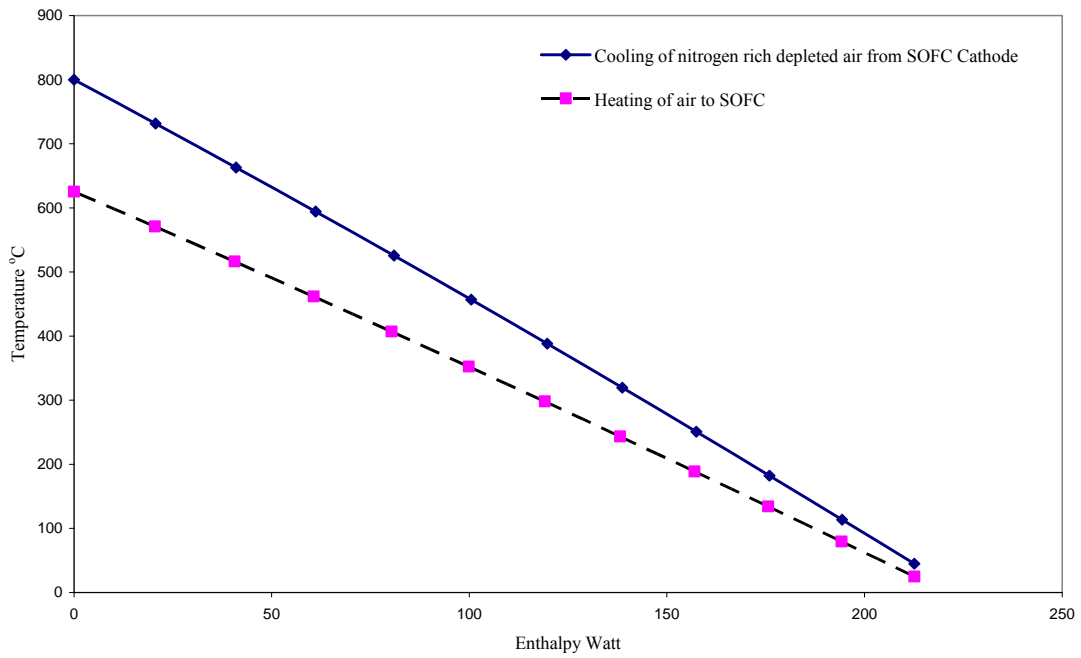


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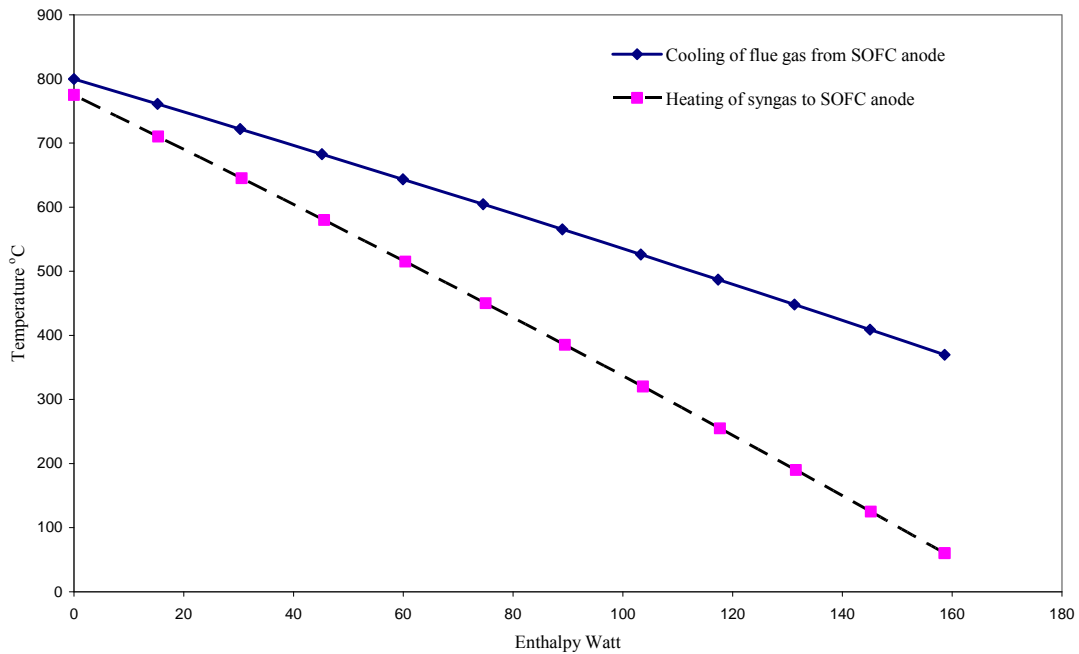
Fig. 4. Aspen simulation of SOFC micro-CHP system (B3 and N2-AIR: preheating of air (AIR2CATH) with nitrogen rich depleted air (NITROGEN); B4 and FLUE-FUE: preheating of syngas (SYN2SOFC) with the flue gas from the SOFC (SOFCFLUE); CATHODE and ANODE are the SOFC cathode and anode respectively; SUPLFIRE: supplementary firing with excess syngas (15); B6: recovery of sensible heat from the SOFC flue gas (FLUE2COOL) into cooling water (12); B7: recovery of heat of condensation and condensate from the remaining dry exhaust gas (10); 11: Hot water recovered from the SOFC flue gas.

The temperature vs enthalpy curves of the two preheaters of air and syngas by the nitrogen rich depleted air and flue gas from the cathode and anode respectively using a minimum temperature approach between the hot and cold streams in Option 1 are presented in Fig. 5. The minimum temperature approach of 20°C for the air preheater exists at the inlet of the air (25°C) and at the outlet of the nitrogen rich depleted air (45°C). For the syngas preheater, the minimum temperature approach arises at the outlet of the syngas and at the inlet of the flue gas, 775°C and 800°C respectively. The (mixed) flue gas condenser has been modeled as an exchanger (with cooling water supplied at 20°C) and a flash separator, B6 and B7 in Aspen simulation in Fig. 4, with outlet temperatures at 60°C and 58°C, respectively. A flash separator was used to separate or recover hot water from the remaining stack gas into the supply of domestic hot water. In an actual implementation, B6 and B7 in Fig. 4 can be combined into one condenser in Option 1, as shown in Fig. 4.

In order to predict the amount of power generation from a SOFC, a steady state irreversible model in Eqs. 1-4 was used<sup>19</sup>. In a fuel cell, chemical reaction energy is converted into electrical energy by consuming hydrogen-rich fuel and oxidant. An Aspen simulation of the SOFC was used to establish such kinetic reaction parameters to feed to the SOFC electrochemical model that predicts the power generation from the SOFC. These parameters included the composition of the syngas, standard molar enthalpy and entropy changes of the system, provided for the two options in Table 3. The other parameters used in the SOFC electrochemical model (Eqs. 1-4) are given in Table 4<sup>19</sup>.



(a)



(b)

Fig. 5. (a) Preheating of air via maximum heat exchange with nitrogen rich depleted air from the cathode of SOFC, with a minimum 20°C temperature difference between the two; (b) Preheating of SOFC syngas via maximum heat exchange with flue gas from the anode of SOFC, with a minimum 25°C temperature difference between the two.



Table 3. Input parameters from Aspen simulation to SOFC's electrochemical model

Mol fraction	Syngas to anode	Oxygen to anode	Flue gas from anode	Change
H <sub>2</sub> O	0.01	0.00	0.46	
N <sub>2</sub>	0.17	0.00	0.17	
O <sub>2</sub>	0.00	1.00	0.00	
H <sub>2</sub>	0.44	0.00	0.00	
CO	0.22	0.00	0.00	
CO <sub>2</sub>	0.15	0.00	0.38	
CH <sub>4</sub>	0.01	0.00	0.00	
Option 1				
Total Flow kmol/hr	0.024	0.00875	0.0248	
Enthalpy J/mol	-61443.909	19187.489	-223371.943	-170691.074
Entropy J/mol °C	43.359	34.492	40.313	-13.809
Option 2				
Total Flow kmol/hr	0.0258	0.0091	0.0263	
Enthalpy J/mol	-70426.953	12101.013	-226505.027	-161604.03
Entropy J/mol °C	33.534	25.505	39.782	-1.939

Table 4. SOFC operating conditions and performance-related parameters<sup>19</sup>, unless generated from Aspen simulation

Parameters	Value
Operating pressure, $p_0$ (bar)	1
Fuel composition, $p_{H_2}$ ; $p_{H_2O}$	From Aspen*
Air composition, $p_{O_2}$ ; $p_{N_2}$	0.21; 0.79
Charge-transfer coefficient, $\beta$	0.5
Number of electrons, $n_e$	2
Pre-factor for anode exchange current density, $\gamma_a$ (A/m <sup>2</sup> )	$5.5 \times 10^8$
Activation energy of anode, $E_{act,a}$ (J/mol)	$1.0 \times 10^5$
Pre-factor for cathode exchange current density, $\gamma_c$ (A/m <sup>2</sup> )	$7.0 \times 10^8$
Activation energy of cathode, $E_{act,c}$ (J/mol)	$1.2 \times 10^5$

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Electrolyte thickness, $L_{el}$ ( $\mu$ m)	20
Activation energy of $O^{2-}$ , $E_{el}$ (J/mol)	$8.0 \times 10^4$
Pre-factor of $O^{2-}$ , $\sigma_0$ (S/m)	$3.6 \times 10^7$
Ratio of the internal resistance to the leakage resistance, $k$	1/100
Anode limiting current density, $i_{L,a}$ ( $A/m^2$ )	$2.99 \times 10^4$
Cathode limiting current density, $i_{L,c}$ ( $A/m^2$ )	$2.16 \times 10^4$
Faraday constant, $F$ (C/mol)	96485
Universal gas constant, $R$ (J/(mol K))	8.314
Standard molar enthalpy change at 1073K, $\Delta h^\circ$ (J/mol)	From Aspen*
Standard molar entropy change at 1073K, $\Delta s^\circ$ (J/(mol K))	From
*Derived in Table 3	Aspen*

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The model adopted for the SOFC is an irreversible and steady state model, in which the irreversibilities resulting from electrochemical reaction, electrical resistance and heat transfer to the environment were taken into account<sup>20</sup>. In addition, the following assumptions were made in this model: fuel compositions in the anode inlet consist of hydrogen, carbon monoxide, methane, nitrogen, carbon dioxide and water vapor mixture, amongst which the first three species participate in the reaction, although the oxidation of hydrogen is much faster than the other two (Table 3). This is a valid assumption as the composition of other components present in the syngas is less than 1 ppm as shown in Fig. 2. In our model we have taken account of all the reacting species in the place of partial pressure of hydrogen and non-reacting species to replace the partial pressure of steam,  $P_{H_2}$  and  $P_{H_2O}$ , respectively. The enthalpy and entropy changes are

corrected accordingly using Aspen simulation results. The SOFC's output voltage is less than the reversible cell voltage because there are some voltage drops across the cell caused by irreversible losses. The electrochemical model takes account of these losses, due to overpotential, or polarization, including three main sources: activation, ohmic and concentration overpotential. In terms of thermodynamic descriptors of the SOFC system, the Gibbs free energy and enthalpy changes were developed for electrochemical reactions, which accounted for both the electrical as well as chemical parameters (Tables 3-4).

It can be noted that the enthalpy and entropy changes obtained from Aspen simulation (Table 3) reflect the nature of the chemical reactions occurring within the anode of the SOFC system at the given temperature and pressure conditions (Table 1) and given compositions of the syngas and air inputs to the SOFC (Fig. 2). The total enthalpy change of the SOFC is divided into electrical and thermal energies. So long as the enthalpy change is more negative than the Gibbs free energy change of the reaction, a part of the total energy is released as heat. This part is a measure of the entropy loss or irreversibility of the SOFC system. Once all these entropy losses (henceforth power losses due to irreversibilities) are calculated, the net power generation is predicted from the difference between the theoretical or thermodynamically maximum power generation and the power losses due to irreversibilities. The final equations derived this way to predict the power generation (in Watt) and efficiency of a SOFC are as in Eqs. 1-2<sup>19</sup>.

$$P_{fc} = \frac{iA}{n_e F} \left( m - \frac{k}{RTd_1} m^2 \right) \quad (\text{Eq. 1})$$

$$\eta_{fc} = \frac{P_{fc}}{-\frac{iA}{n_e F} \Delta h^\circ} = \frac{1}{-\Delta h^\circ} \left( m - \frac{k}{RTd_1} m^2 \right) \quad (\text{Eq. 2})$$

Where  $d_1 = 2n_e \sinh^{-1}\left(\frac{i}{2i_{0,a}}\right) + 2n_e \sinh^{-1}\left(\frac{i}{2i_{0,c}}\right) - \ln\left(1 - \frac{i}{i_{L,a}}\right) - \ln\left(1 - \frac{i}{i_{L,c}}\right) + \frac{i n_e F L_{el}}{\sigma_0 R} \exp\left(\frac{E_{el}}{RT}\right)$ ,  $k = R_{int} / R_{leak}$ , and

$$m = -\Delta h^\circ + T\Delta s^\circ + RT \ln\left(\frac{p_{H_2} p_{O_2}^{1/2}}{p_{H_2O}}\right) - RT d_1.$$

The terms in  $d_1$  from left hand side to right hand side indicate the voltage drops across anode and cathode caused by activation overpotential (the first two terms), concentration overpotential (the second two terms) and Ohmic overpotential (the last term) respectively.  $i$  is the current density,  $F = 96,485 \text{ C mol}^{-1}$  is Faraday's constant,  $R = 8.314 \text{ J mol}^{-1} \text{ K}^{-1}$  is the universal gas constant.  $n_e$  is the number of electrons participating in the reaction.  $A$  is the surface area of the fuel cell polar plate,  $\Delta h^\circ$  and  $\Delta s^\circ$  are the standard molar enthalpy and entropy changes of the reaction at temperature  $T$ , respectively,  $k$  denotes the ratio of the equivalent leakage resistance to the internal resistance of the fuel cell and is assumed to be a constant.  $L_{el}$  is the thickness of electrolyte,  $E_{el}$  represents the activation energy for ion transport, and  $\sigma_0$  is the reference ionic conductivity.  $p_0$  is the ambient pressure,  $p_{H_2}$ ,  $p_{O_2}$  and  $p_{H_2O}$  are the partial pressures of reactants,  $O_2$  and non-reacting components, respectively.  $i_{L,a}$  and  $i_{L,c}$  are the limiting current densities of the anode and cathode, respectively. The anode and cathode exchange current densities,  $i_{0,a}$  and  $i_{0,c}$ , are calculated using Eqs. 3-4<sup>19</sup> respectively and the rest of the parameters present in Eqs. 1-2 is either fixed values or obtained from Aspen simulation, provided in Tables 3-4. Table 4 also contains the nomenclature of the parameters used.

$$i_{0,a} = \gamma_a \left(\frac{p_{H_2}}{p_0}\right) \left(\frac{p_{H_2O}}{p_0}\right) \exp\left(-\frac{E_{act,a}}{RT}\right) \quad (\text{Eq. 3})$$

$$i_{0,c} = \gamma_c \left(\frac{p_{O_2}}{p_0}\right)^{1/4} \exp\left(-\frac{E_{act,c}}{RT}\right) \quad (\text{Eq. 4})$$

$\gamma_a$  and  $\gamma_c$  are pre-exponential coefficients for the anode and cathode, respectively.  $E_{act,a}$  and  $E_{act,c}$  are activation energies for the anode and cathode, respectively.

A comparison of energetic analysis between the two SOFC design options obtained from combined Aspen simulation and electrochemical modelling, is presented in Table 5. The heat transfer related results, such as heat duties of exchangers, outlet temperatures of either of the hot or cold streams, log mean temperature differences (LMTD), overall heat transfer coefficients (U) and heat exchanger areas, as provided in Table 5 were established using Aspen simulations. The total residential heat supply consists of the total sensible plus condensation heat recovered from the (mixed) flue gas from the SOFC (Fig. 3 or (mixed) flue gas cooler and phase separator, B6 and B7 respectively in Aspen simulation in Fig. 4) as well as the condensate recovered as domestic hot water from the remaining stack gas. The sensible heat and the heat of condensation of the (mixed) flue gas from the SOFC recovered into cooling water circulated as a source of residential heat are 0.172 kW<sub>th</sub> and 0.035 kW<sub>th</sub> in Option 1 and 0.229 kW<sub>th</sub> and 0.122 kW<sub>th</sub> in Option 2, respectively. The balance of the total residential heat generation reported in Table 5 indicates the heat recovered via condensate from the remaining dry stack gas. The heat exchanger details for the sensible heat recovery from the flue gas to 60°C were only reported in Table 5 for a comparison purpose between the two options.

Table 5. Comparison of energetic analysis between the maximum and co-current preheating design options of SOFC based micro-CHP system

Heat exchanger units	Air preheater	SOFC fuel gas preheater	Exhaust cooler
Hot stream	N <sub>2</sub> rich depleted air from SOFC cathode	Flue gas from SOFC anode	(Mixed) flue gas from SOFC
Cold stream	Air to SOFC cathode	Fuel gas to SOFC anode	Cooling water for residential heat
<b>Option 1</b>	Minimum temperature driving force / maximum heat recovery in preheaters / maximum SOFC power generation		
Hot side temperatures °C	Hot stream / Cold stream: 800 / 625.5	800 / 775	369.6 / 70
Cold side temperatures °C	45 / 25	369.6 / 60	60** / 20
Heat duty kW <sub>th</sub>	0.2126	0.1586	0.1722*
Area m <sup>2</sup>	0.0035	0.0016	0.0016
U W/m <sup>2</sup> K	850.00	850.00	850.01
LMTD °C	71.32	113.10	128.93
Total area m <sup>2</sup>		0.0067	
SOFC power kW <sub>e</sub>		1.00	
SOFC current density A		13.14	
Total residential heat kW <sub>th</sub>		0.21	
Power to heat ratio %		82.34	
<b>Option 2</b>	Cocurrent preheaters with minimum temperature approach		
Hot side temperatures °C	Hot stream / Cold stream: 800 / 415	800 / 517	467 / 70 (countercurrent)
Cold side temperatures °C	435 / 25	537 / 60	60** / 20 (countercurrent)
Heat duty kW <sub>th</sub>	0.1206	0.0945	0.2291*
Area m <sup>2</sup>	0.0004	0.0003	0.0019
U W/m <sup>2</sup> K	850.00	850.00	850.01
LMTD °C	397.37	371.55	141.48
Total area m <sup>2</sup>		0.0026	
SOFC power kW <sub>e</sub>		1.00	
SOFC current density A		26.30	
Total residential heat kW <sub>th</sub>		0.36	
Power to heat ratio %		73.65	

\*\*Just above the dew point

\*Contributed to residential heating via generation of hot water at 70°C

The electrochemical modelling of a SOFC established the current density and area required,  $i \times A$  (current density in A/m<sup>2</sup> × cell area in m<sup>2</sup>) equal to 13.14 A and 13.17 A, for 1 kW<sub>e</sub> power generation from the two SOFC design options, respectively. The syngas fuel requirements in Options 1-2 are 0.4515 kg/hr and 0.4851 kg/hr respectively, based on 85% fuel utilisation efficiency in the SOFC anode. Due to the maximum preheating of the SOFC feed gases in Option 1, less syngas is required to generate the same amount of enthalpy or exothermic heat of reaction from the SOFC anode, as obtained from the Aspen simulation. This value is between 1.176-1.181 kW<sub>th</sub> (Table 3) for a generation of 1 kW<sub>e</sub> of electricity. From Table 5, it can also be demonstrated that 0.15 kW<sub>th</sub> of increased preheating can be made available for power generation from the SOFC in Option 1, resulting in a ratio of 82.34% of electricity to heat generation. While this amount of heat is utilised in residential heating in Option 2, providing a 73.65%

share of electricity out of the total energy generation from the SOFC. This higher electrical to heat generation efficiency from Option 1 is obtained at the cost of 0.0273 m<sup>2</sup>/kW of more exchanger area and lower residential heating rate. The total energy generation from Options 1-2 is 1.21 kW and 1.36 kW respectively (Table 5).

#### **4. Integration of SOFC systems with other renewable technologies in the context of UK residential energy demands**

This study takes the high UK residential heat demand analysis into account<sup>10-14</sup> and endeavors to integrate SOFC based micro-CHP systems with heat led renewable technologies, so as to closely match with the UK residential heat requirements. A straightforward solution is the generation of additional heat using supplementary firing in a burner or boiler, utilising the same fuel, syngas. Further, Aspen simulation revealed that a supply of 2.2 times more syngas than that required for the SOFC micro-CHP can fulfill the balance of heat demand by the UK residential sector. The heat generation from a supplementary firing of 0.9933 kg/hr of syngas is 2.35 kW<sub>th</sub> based on 90% efficiency of the boiler, totaling to 2.56 kW<sub>th</sub> of heat or 72% of heat to power generation ratio from Option 1. On supplementary firing the overall CHP generation efficiency from Option 1 was 82.7% based on HHV of syngas (4.31 kW or 1.445 kg/hr).

The GSHP can also provide effective solutions to residential heating / cooling applications. The GSHP works on heat pump or refrigeration principle, in which the solar energy stored in the ground is absorbed via evaporation or heating of a refrigerant at low pressure, followed by compression of the refrigerant vapour. The high pressure and high temperature refrigerant vapor is then condensed or cooled providing residential heating, expanded and sent back to extract heat from the ground. Fig. 6 presents a coupled GSHP refrigeration cycle and SOFC. The cycle can also be operated to provide cooling instead of heating.

The technology exploits the fact that the temperature of the earth at moderate depth is slightly higher in winter than the air temperature at the surface (and in summer slightly lower)<sup>15</sup>. In the UK, ground temperatures stay fairly constant, between 10°-14°C, throughout the year<sup>15</sup>. A SOFC and GSHP have thermodynamic integration synergy between them. However, no demonstration result has been published yet<sup>15</sup>. The high pressure and high temperature condensation / cooling part of a GSHP cycle can be replaced by a pressurised SOFC, as illustrated in Fig. 7.

Studies have demonstrated the application of conceptual heat integration and analysis tools for providing condensation heat for gas separation systems from refrigeration systems<sup>16</sup>. Novel designs and operability for ethylene plant were also deduced using conceptual programming<sup>17</sup> and more recently multi-objective optimization<sup>30</sup>. Such studies can become highly important and relevant for more detailed integrated renewable energy system designs, considered in the report of Energy Saving Trust<sup>15</sup>. For establishing the thermodynamic efficiency of the integrated SOFC-GSHP system, a conceptual process configuration coupling a pressurised SOFC within a GSHP, depicted in Figs. 6-7, has been generated using heat integration in Aspen Plus. The integration concept lies in the utilization of the high pressure and high temperature exhaust gas from a SOFC as a refrigerant in a GSHP loop. A water/anti-freeze mixture can be used as the refrigerant in a GSHP. The (mixed) flue gas from a SOFC using syngas as fuel comprised of nitrogen (63% by mole) and carbon dioxide (16% by mole) as the main constituents with the balance being water and thus inherently exhibits properties of refrigerant. An essential difference between this option and the two options explored for standalone application of SOFC micro-CHP is that the heat from the SOFC exhaust gas is extracted at high pressure (5 bar), leading to condensation of the gas, in 'SOFC exhaust gas condenser' in Fig. 6 or in exchanger B6 and cooler B3 in Aspen simulation in Fig. 7, respectively. The two phase stream is then expanded through the expansion valve in Fig. 6 or B8 in Fig. 7, respectively, to atmospheric pressure, sent to below the ground surface to extract heat (in the evaporator in



Fig. 6 or in GSHP in Aspen simulation in Fig. 7, respectively assuming 10°C temperature difference from the ground heat) and compressed back to the high pressure and high temperature, 5 bar and 60°C, through the compressor in Fig. 6 or B7 in Aspen simulation in Fig. 7, respectively, ready to provide residential heat. Instead of closing the loop, the two phase system, water phase and a gas phase with nitrogen and carbon dioxide as the main constituent, can be released to atmosphere, after residential heat recovery (from B10-B11 in Fig. 7) in order to continuously operate the SOFC. The SOFC's role in this case is to provide high pressure, compressor duties and refrigerant for GSHP.

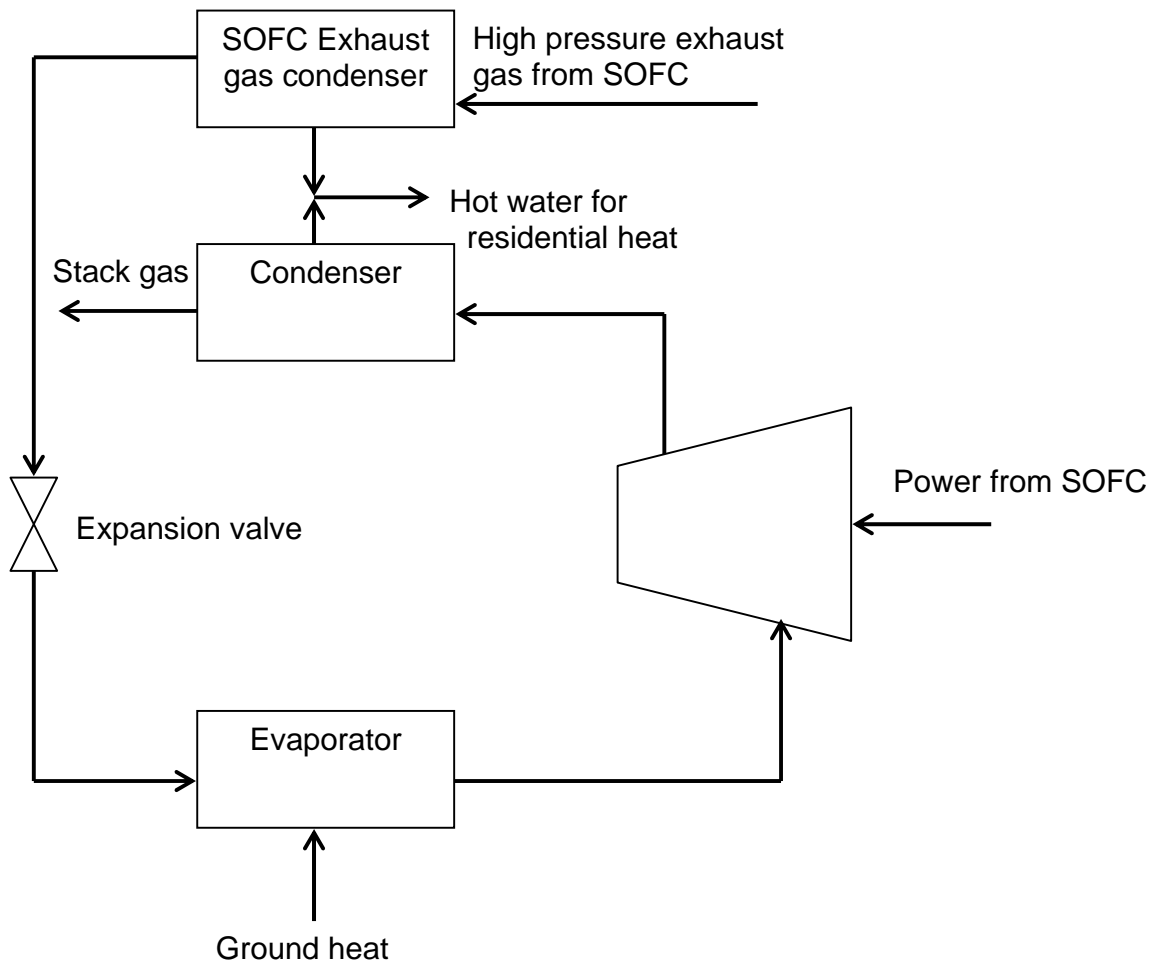


Fig. 6. Proposed integration between SOFC and GSHP systems.

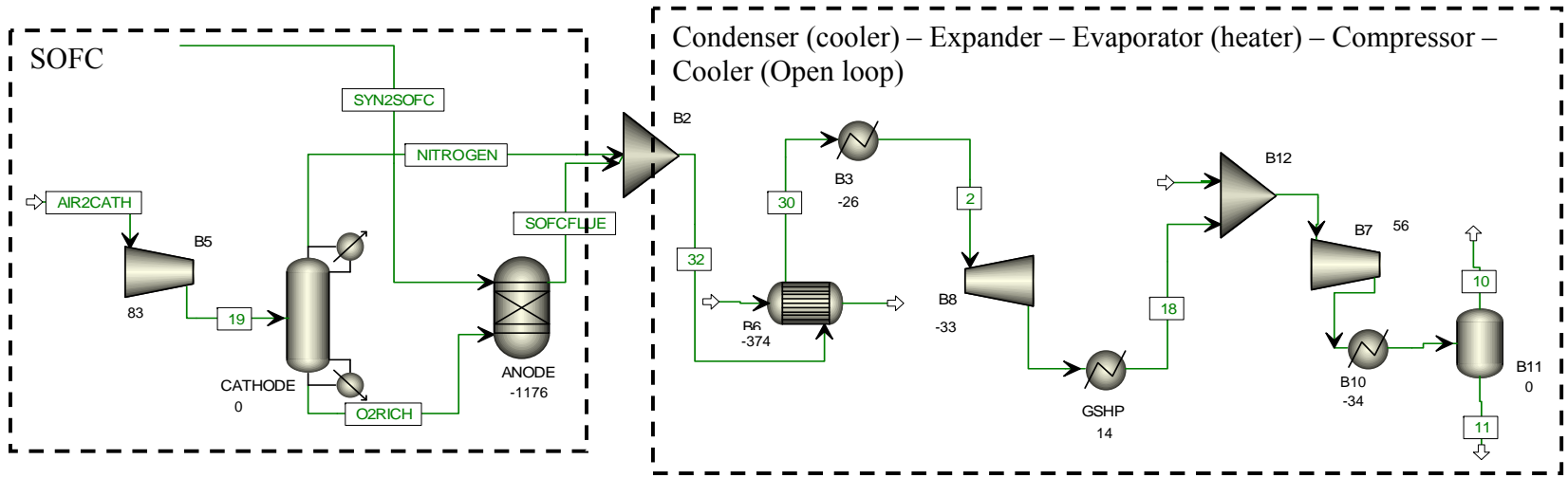


Fig. 7. Aspen simulation of integrated SOFC-GSHP micro-CHP system (heat and power generation and consumption shown are in kW).

The pressurised SOFC systems have been demonstrated at kW<sup>31</sup> as well as at MW scale<sup>32</sup>. Based on 1 MW<sub>e</sub> power generation and 85% fuel utilization efficiency from the SOFC, the syngas flowrate needs to be 536 kg/hr. Hence, for the given configuration of the straw based gasification plant (Fig. 2), a minimum straw slurry flowrate of 372 kg/hr will be required to generate 1 MW of power from the SOFC. For the same straw slurry flowrate, the equivalent power generation from gas turbine based combined cycle is 411 kW<sub>e</sub>. Considering the scale of electricity production, it is thus more rational to exploit the integrated SOFC-GSHP system for community-scale generation, rather than residential micro-CHP. Furthermore, the vertical or horizontal GSHP loops require a significant amount of space underground<sup>30</sup>. Thus, the hybrid SOFC-GSHP system becomes more applicable to community-scale energy supply.

The net power generation from the SOFC-GSHP system includes the output power generation from SOFC (1 MW<sub>e</sub> output based on 85% of exothermic heat of reaction reported in Fig. 7) and expander (33 kW<sub>e</sub>) and input power consumption by air compressor (83 kW<sub>e</sub>) and (mixed) flue gas compressor (56 kW<sub>e</sub>). The net heat generation is obtained by subtracting the ground source heat extracted (GSHP: 14 kW<sub>th</sub>) from the heat generation by the condenser (374 kW<sub>th</sub>) and the coolers (26 kW<sub>th</sub> and 34 kW<sub>th</sub>), respectively (Fig. 2). The amount of power generation is 68% of the total energy generation. The high power density of SOFC and thereby low flowrate of the resulting exhaust gas per unit electricity produced results in relatively less amount of heat extraction from the ground. Even then, a higher efficiency of ~90% can be achieved from the overall integrated SOFC-GSHP system proposed (Fig. 7). Selection and mixing of more suitable refrigerants into the SOFC exhaust gas should be explored for a thermodynamically optimal integration between SOFC and GSHP micro-CHP, subject to further research, when the results from the first demonstration plant would be available.

Similar to GSHP, heat available in the air can also be utilized in the heat pump (Air Source Heat Pump, ASHP) and to increase the residential heating rate. Thus, an air intake to the compressor B7 was considered to increase the heat recovery rate through B10 (Fig. 7). However, this route neither utilizes the high pressure and high temperature advantages of the SOFC process nor contributes to the exhaust gas refrigerant medium. The only connection between ASHP and SOFC systems is via the supply of the power requirements by the ASHP system from SOFC. Thus, integration in this line lowers the overall efficiency. For example, based on an air flowrate of 0.32 kmol/hr (with referenced to 0.024 kmol/hr of syngas flowrate to SOFC in Table 3) a desirable heat to power ratio of 68% for the UK new residential systems was obtained, however this results in an overall reduced efficiency to 83% due to the conversion of electrical energy into thermal energy.

It is expected that during summer months when there is low or no heat demand, SOFC-supplementary firing and SOFC-GSHP systems can be designed to meet the lowest heat requirement. During peak heat demands these systems can rely upon thermal storage systems<sup>13</sup> and / or other form of renewable technologies for dwellings (e.g. solar heat) or community based generations (such as the biomass waste based gasification combined cycle plant studied here). If surplus electricity is generated, the basic options are to, sell it directly to customers or to the grid. A straightforward way can be by net metering, where the electricity exported is subtracted from the fuel or CHP imported, with only the balance being paid for.

## **5. Conclusions**

The integrated energy systems design may be undertaken between community and individual dwelling level CHP generations (different scales) and may also call integration between heat and power led CHP generation technologies. Integrated energy systems are technologically more viable compared to stand-

alone processes. Thermodynamic feasibility in terms of heat integration must be established using conceptual design frameworks in order to demonstrate increased energy efficiency from energy systems integration. In the context of the UK residential sector, the heat-led micro-CHP has been a focal point of research. However, heat-led CHP technologies may result in intermittent supply of electricity during summer months. A SOFC based micro-CHP system can achieve a very high energy generation efficiency compared to conventional gas turbines. By developing novel energy integration strategies, A SOFC can further be used flexibly to fulfill the high heat demand by the UK residential sector. In this paper, the technical feasibility of integration of SOFC based micro-CHP systems with a renewable feedstock, syngas derived from straws, was investigated. The study looks into the integration between a community-scale waste derived syngas (50-100 kW<sub>e</sub> of electricity using gas turbines) and SOFC based micro-CHP installation in individual dwellings (1 kW<sub>e</sub> of electricity from SOFC). The process design approach comprised of heat integration and integrated flowsheet simulation in Aspen Plus. Furthermore, integration between SOFC and heat-led renewable energy technologies, such as syngas boilers, GSHP and ASHP, was considered to regulate the micro-CHP generation in the face of the UK residential heat and power demands. Five major energy systems have thus been presented as viable integrated community-scale and micro-CHP energy technologies: 1) biomass gasification plant utilizing straws into community-scale CHP generation for dwellings; 2) SOFC based micro-CHP; 3) SOFC-syngas boiler based micro-CHP; 4) integrated SOFC and GSHP system and 5) integrated SOFC and ASHP system. The last four options used syngas from community-scale biomass gasification plant. In summary, it is recommended that SOFC based micro-CHP systems should be operated at the highest electrical efficiency utilizing maximum energy integration and the balance of the heat requirement should be fulfilled by energetic integration with the heat-led renewable technologies.

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