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Optimisation of an SOFC/GT system with CO₂-capture

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Abstract

Hybrid systems combining solid oxide fuel cells and gas turbines (SOFC/GT) have been extensively studied in recent years. They show very high theoretical electrical efficiencies and are considered as prime contenders for distributed generation. The addition of a CO_2 -capture system could make them even more attractive from an environmental perspective. In this study, a SOFC/GT configuration with and without a tail-end CO_2 separation plant has been examined.

In this work, the key parameters of the hybrid system are selected by an innovative tool based on a genetic algorithm (GA), which replaces the cumbersome parameter studies that generally are performed for this purpose. The focus is put on the evaluation of the GA as a tool for handling the multi-variable non-linear optimisation problem. The result of the optimisation procedure is a SOFC/GT system that exhibits an electrical efficiency above 60% with part capture of the CO_2 .

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1. Introduction

The increased availability and use of natural gas as a primary energy source in conjunction with the deregulation of the electricity market are promoting distributed generation (DG), whose share of energy will be important in the future years [1,2]. Certainly there is no unique definition for DG, but general consensus seems to address that DG is power or combined heat and power (CHP) generating units with no central planning, no central dispatch, connected close to the load (i.e. on the distribution network or on the customer side of the meter), and with rating smaller than 50-100 MW [3]. DG can also refer to facilities in remote places with no power grid where they are the only power source [4]. Stand-alone fuel cells, or fuel cells in combination with gas turbines, fit into the characteristics described above and are therefore considered as an attractive alternative for DG. The higher theoretical electrical efficiency of these hybrid systems, together with the use of natural gas, make them interesting from an environmental point of view. The addition of a tail-end CO₂ separation plant would make these plants even more environment-friendly.

However, to establish an optimal SOFC/GT system at a pre-design level implies the specification of different parameters usually found by cumbersome parameter variations. Depending on the complexity of the model, as many as 5 to 10 (or even more) independent parameters can be involved in the study, making the correlation between them unclear. The addition of further components, such as a CO_2 separation plant, would increase the difficulty of this procedure. Therefore, an innovative optimisation technique that can handle these non-linear multi-dimensional systems, known as genetic algorithms (GA), is addressed in this work. The focus is put on the evaluation of this tool for the SOFC/GT system optimisation problem.

2. Previous research related to this work

In the field of optimising SOFC/GT hybrid systems, little has been done. Variations of process parameters have been performed by both Pålsson [5] on SOFC/GT systems and Riensche et al. [6] on atmospheric systems. These studies are limited to the variation of one parameter at a time:

• Pålsson chose to vary stack size, pressure ratio, steam-to-carbon ratio, recuperator efficiency and the fuel split between fuel cells and supplementary firing, keeping the turbine inlet temperature (TIT) constant.

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Nomenclature			
CHP	combined heat and power		
DG	distributed generation		
GA	genetic algorithm		
MEA	monoethanolamine		
SOFC/GT	solid oxide fuel cell and gas turbine		
TIT	turbine inlet temperature		
$n_{\rm f}^{\rm in}, n_{\rm f}^{\rm out}$	molar flow rates of inlet and outlet fuel species at stoichiometry		
U_{f}	fuel utilisation factor		

• Riensche et al. varied cell voltage, fuel utilisation, degree of pre-reforming and air temperature increase in the stack, while the stack size was adjusted.

Clearly, there is a need for a tool or an algorithm capable of evaluating several parameters at a time, and GA is believed to be such a tool.

Optimisation can also be performed as a modification of the system configuration, e.g. anode/cathode gas recycling, networking of fuel cell stacks, etc. These features are considered out of the scope of the present work; therefore the system configuration is kept unchanged.

Studies of SOFC with CO₂-capture have been performed earlier by many researchers. An excellent overview of the different concepts is given by Dijkstra and Jansen [7]. They present a classification dividing the different systems in pre-combustion CO₂-capture, post-combustion CO₂-capture and post-combustion off-gas treatment, with a novel contribution of their own based on hydrogen-selective membranes. Of particular interest is also the SOFC system with an "afterburning" section presented by Siemens Westinghouse and Shell, which indicates electrical efficiency up to 70%, if the system is pressurised and operated in a hybrid mode with a gas turbine [8].

3. Genetic algorithms

The term genetic algorithm (GA) refers to a large class of heuristic search techniques which identify improved solutions by mimicking the biological processes of natural selection by "survival of the fittest". This method, pioneered by Holland [9], has three basic components: a *population* of possible solutions to the problem, a criterion to rank the *fitness* of different solutions, also known as an *objective function*, and a way to breed new solutions. The best solutions giving the highest fitness are chosen to survive and recombine with each other to produce the next generation of possible solutions. It is expected that the fitness should increase with each new generation. Techniques to include solutions not found in the starting population, such as *mutation*, also exist. GA methods are very robust and do not show the susceptibility to entrapment by local optima that is typical of calculus-based methods [10]. For thermodynamic applications such as a power plant optimisation, the optimiser may adjust a number of *decision variables* defining crucial design parameters for the plant within specified ranges, whilst the objective function can be the thermal efficiency or the cost of electricity.

The specific GA method used in this paper represents the search interval of each decision parameter by a binary number; 8 bits being generally adequate for engineering purposes. These binary numbers are then joined to form a string unique for each particular combination of cycle parameters. The initial population is generated by random distribution over the prescribed ranges of the decision parameters. To choose the fittest members in the population, a tournament selection approach is used [11]. The specific method used here randomly chooses three members at a time from the current population, then passes the fittest of these to a mating pool. This process is repeated until enough members have been selected for the pool. Successive pairs of solutions are then randomly drawn from this mating pool and either "mated" to produce two new solutions for the next generation, or passed unchanged to the next generation, thus saving some of the good solutions depending on a specified *crossover probability*. In single point crossover, the binary string representations of the two parents are cut at some random position, and the final sub-strings are interchanged to produce two new "child" strings. Mutation is a secondary operator that introduces a small probability that part of the coding of any new "child" string may be deliberately changed to maintain diversity of the population. Each child string is then decoded to produce the physical decision parameters for the new population member. For a detailed description of different GA methods, see the textbooks by Holland [9], Goldberg [10] and Mitchell [11].

4. SOFC model

A model based on the finite volume method has been developed by Selimovic [12] for simulation of a planar SOFC with internal reforming. The model has been used extensively in simulations of hybrid SOFC/GT cycles and is described elsewhere [5,12]. The operating characteristics of a single cell have been predicted, i.e. gas utilisation, electric power, energy efficiency, species concentration and current and temperature distribution. Conservation equations have been formulated for the solid part of the cell and for the gas channels. The results from this two-dimensional steady-state model were compared with other models in a benchmark test showing good agreement [13]. The stack model used in the system models are represented as a multiplication of single cells. This two-dimensional approach using cell voltage and number of cells as input has been compared to a three-dimensional model with satisfactory results [12].

A fuel utilisation factor (U_f) of the cell is defined in Eq. (1), where *n* denotes the molar flow rates of inlet and

outlet fuel species at stoichiometry (higher hydrocarbons are converted in a pre-reformer, if present). A practical maximum for the fuel utilisation is between 80 and 90% [14].

$$U_{\rm f} = \frac{n_{\rm f}^{\rm in} - n_{\rm f}^{\rm out}}{n_{\rm f}^{\rm in}} \tag{1}$$

where $n_{\rm f} = n_{\rm H_2} + n_{\rm CO} + 4n_{\rm CH_4}$.

5. Techniques for abatement of CO₂ emissions

Carbon dioxide has been identified as a major greenhouse gas responsible for over half of the increase in global warming [15]. The combustion of fossil fuels is the largest contributor to CO_2 emissions, especially in the field of power generation, but also in the transport sector. Increases in the global surface temperature (0.3–0.6 °C) and the sea level (10–25 cm) over the last 100 years has already been documented and are strongly believed to be inflicted by man [15].

The carbon dioxide problem can be dealt with in various ways. A more efficient way of using and producing energy will obviously lead to lower CO_2 emissions. Also, a shift toward fuels with low carbon content, such as natural gas, or renewable fuels with no net release of CO_2 is desirable. However, for many applications an immediate choice is the capture of CO_2 from the flue gases, so-called post-treatment. Here chemical absorption can be mentioned, which is perhaps one of the most accepted techniques today. A description of post-treatment methods for CO_2 recovery as well as a summary of the effects on economy and efficiency can be found in [16].

Other ways of capturing CO_2 include O_2/CO_2 firing in which pure oxygen is used for combustion requiring an air separation unit, and CO shift in which the CO_2 is separated by physical absorption from a reformed and gas-shifted syngas fuel before combustion. The efficiency penalty of these CO_2 -reducing technologies have been calculated to be between 7 and 12 percentage points, respectively, whereas the cost of electricity is estimated to increase by between 20 and 60% [17]. A fourth possibility is to use processes in which the fuel and air do not come into direct contact, such as chemical looping [18,19], where oxygen in the combustion air is transferred to the fuel via particles of metal/metal oxides and of course fuel cells, which is the subject of this work [5,12].

 CO_2 removal includes many steps such as recovery, transportation and utilisation, storage or disposal. Ideally, CO_2 should be dried from water and liquefied for making the transportation easier, or solidified at low temperatures (-78 °C, 1 atm). This work does not cover these removal steps nor consider their impact on the overall performance.

6. System modelling

Two systems have been studied and optimised in this work; a reference SOFC/GT system and the same system

with a conventional tail-end CO₂ separation plant. Both systems have been modelled using IPSEproTM commercial software for heat and mass balance calculations with an open environment and possibility to include user-specific models. Studies have shown that a gas turbine suitable for a hybrid SOFC/GT system is not available today, i.e. the gas turbine needs to be redesigned [20]. Therefore, a generic GT-model has been used in this study.

The reference SOFC/GT system consists of a two SOFC stacks topping a recuperated gas turbine cycle (see Fig. 1). Pure methane (CH_4) is used as fuel, which is heated and desulphurised before it is mixed with steam and supplied to a pre-reformer. The steam-to-carbon molar ratio is set to 2.0, as low as possible considering the risk for carbon deposition. The main fuel stream is equally split between the two stacks, i.e. the fuel side is connected in parallel. On the air side, the stacks are connected in series. Each stack has 7500 cells. The fuel utilisation is maximised to 85% in each cell and the rest of the fuel is burned in the gas turbine combustor with supplementary fuel supply. To avoid the need for cooling in the gas turbine expander, the maximum TIT is set to 950 °C. In the fuel cell stacks the material temperature is limited to 1050 °C. A district heating system makes use of the low-temperature heat left in the exhaust gases after the recuperator. A summary of the assumptions for the reference system can be found in Table 1.

In the SOFC/GT system with CO₂-capture, the flue gas is cooled and dried in an exhaust gas condenser. Eventually, the CO₂ in the flue gas stream is separated by means of chemical absorption using monoethanolamine (MEA) as absorbent. A calculation model for this post-treatment CO₂ separation plant has been implemented in IPSEproTM. The outline of the CO₂ separation model can be found in the textbook by Kohl and Nielsen [21], here implemented with simplifications for flue gases without hydrogen sulphide, H₂S.

The objective of the CO_2 separation model is to predict the steam consumption for regeneration of the amine solution at a given regeneration temperature. For this purpose, the needed input information is the flue gas composition,

Table 1						
Calculation	assumptions	for	the	reference	SOFC/GT	system

Number of cells in each stack	7500
Desulphurisation temperature (°C)	400
Fuel temperature at SOFC inlet (°C)	850
Compressor isentropic efficiency	0.81
Turbine isentropic efficiency	0.84
Generator efficiency	0.98
Combustion efficiency	0.99
Heat exchanger pressure drop (%)	2
Combustor pressure drop (%)	5
Fuel cell stack pressure drop (mbar)	10
dc/ac converter efficiency	0.95
Turbomachinery mechanical efficiency	0.995
Recuperator pinch-point (°C)	30



Fig. 1. System layout for the reference SOFC/GT system.

Table 2Assumptions for the CO2 separation plant

Amine (MEA) concentration (%)	30
Flue gas temperature at absorber inlet (°C)	30
Flue gas pressure drop in exhaust gas condenser (mbar)	10
Flue gas pressure drop in absorber (mbar)	40
Regenerator temperature (°C)	120
Regenerator reflux ratio (mol H ₂ O/mol CO ₂)	0.8
CO ₂ removal degree depends on steam availability	

pressure and flow rate coming from the power plant model. In these calculations it is assumed that the steam for the regeneration of MEA in the CO_2 separation plant is produced with the low-temperature heat available in the flue gases (see Fig. 2). Assumptions for this system are the same as for the reference system above, with the addition of the parameters presented in Table 2.

7. Calculations

All calculations are carried out at design point, i.e. no consideration has been taken to part-load properties of the SOFC/GT system. In the optimisation studies, the electric efficiency is selected as the objective function with the air flow, fuel flows (main and supplementary), cell voltage in the stacks, air temperature at the stack inlet, reformer duty

and pressure ratio as decision parameters. The maximum allowed temperatures in the SOFC stacks and at the turbine inlet were used as constraints, while the stack size was kept constant. Due to the implicit calculation of maximum stack temperature, it was not possible to use it as a decision parameter or a setting. It is well known that the higher the temperature is in the stack, the better the efficiency will be. Instead, the expected result from the optimisation was to find a combination of fuel flows, air flow, air temperature, degree of pre-reforming and cell voltages resulting in the maximum allowable stack temperature and highest electrical efficiency. Decision parameters with variation ranges, convergence ranges and optimal values found by the GA optimiser are shown in Tables 3 and 4 for the reference SOFC/GT system and the system with CO₂-capture, respectively. Several runs of each optimisation case were made and only the best results are shown here.

It was found that the impact of stack temperature was very high in comparison to other parameters. Once a solution had reached the limit of 1050 °C, the optimiser showed difficulties finding other combinations also giving high stack temperature but higher efficiency. Effectively, this means changing at least two other parameters and still having a maximum stack temperature close to 1050 °C, although no higher. The best results were therefore found when the air temperatures to the stack and the cell voltage were set to be equal in both stacks. The performance of the optimised systems is shown in Table 5.



Fig. 2. System layout for the SOFC/GT with CO₂-capture.

Table 3 The decision parameters and optimisation results for the reference SOFC/GT system

Parameter (unit)	Variation range	Convergence range	Best solution
Compressor pressure ratio	2.5–5	2.86–4.91	2.97
Reformer duty (kW)	20-200	23-163	152.4
Cell voltage, stacks 1 and 2 (V)	0.68–0.8	0.686–0.8	0.747
Inlet air temperature, stacks 1 and 2 (°C)	850-950	854–944	921
Fuel flow (kg/s)	0.008-0.013	0.0082-0.0124	0.01086
Supplementary fuel flow (kg/s)	0-0.003	0-0.0027	0
Air flow (kg/s)	0.8–1.2	0.803–1.19	0.803

Table 4

The decision parameters and optimisation results for the SOFC/GT system with CO2-capture

Parameter (unit)	Variation range	Convergence range	Best solution
Compressor pressure ratio	2.5–5	2.5-4.5	3.91
Reformer duty (kW)	20-200	28-102	102
Cell voltage, stacks 1 and 2 (V)	0.68–0.8	0.709–0.8	0.711
Inlet air temperature, stacks 1 and 2 (°C)	850-950	869–937	890
Fuel flow (kg/s)	0.008-0.013	0.0088-0.0127	0.0114
Supplementary fuel flow (kg/s)	0-0.003	0.0001-0.0028	0.00074
Air flow (kg/s)	0.75-1.2	0.778-1.19	0.778

Table 5 Results from the optimised SOFC/GT systems

Parameter (unit)	Reference SOFC/GT system	SOFC/GT system with CO ₂ -capture	
Electrical efficiency (%)	64.6	63.0	
Overall (CHP) efficiency (%)	78.3	63.0 ^a	
CO ₂ removal (%)	_	67	
Degree of pre-reforming (%)	83	53	
Stack temperature, stack 1 (°C)	1049.8	1049.4	
Stack temperature, stack 2 (°C)	1049.5	1049.9	
Turbine inlet temperature (°C)	926	946	
Fuel utilisation factor, stack 1 (%)	75.7	79.0	
Fuel utilisation factor, stack 2 (%)	74.7	78.1	

^a No heat production in this application.

8. Results and discussion

The following conclusions can be drawn from the optimisation calculations. Stack temperature is the parameter influencing efficiency the most. Furthermore, a low air flow and no or little supplementary fuel are also beneficial. However, the supplementary fuel can be important to secure that the off-gases can be burned, especially at part-load operation [22]. Another option in this case is to use a catalytic burner in the gas turbine. The degree of pre-reforming showed a benefit in efficiency at a high percentage; in agreement with Pålsson's results [5] but somewhat contradictive to Riensche et al.'s [6]. One possible explanation could be the level of detail in the models where the model used in this study does take the effect of uneven temperature distribution into account. The other three parameters did not show any conclusive results but rather, seem to have a flat optimum within the evaluated range. Pressure ratio optimum was found at around three for the reference SOFC/GT cycle and close to four for the SOFC/GT cycle with CO_2 -capture. The higher pressure ratio for the CO_2 separated cycle is believed to be caused by the higher pressure drop in the components after the turbine.

The genetic algorithm optimiser, although finding good solutions, showed some difficulties using a combination of constraints and search intervals. This problem could possibly be overcome by using multi-point crossover in the mating process or a very high mutation rate, but this would make the optimisation more time-consuming as it nears a random search process. Another approach that could be helpful would be an even larger population size in combination with a narrowed search interval, although this would also have implications on calculation time. A plot of the progress of a typical GA optimisation can be seen in Fig. 3. Progress is fast in the first 15 generations, but there is still an increase in the best electrical efficiency even after generation 50. The



Fig. 3. Progress of the optimisation.

calculations were performed using a population of 150, calculating for 80 generations with each parameter represented by an 8-bit binary number, thus dividing the interval in 256 different values.

Although the degree of CO₂-capture is not comparable to many other systems (60–70% compared to 90 or 100%), the electrical efficiency of this system is very competitive. For a small industry using CO₂ in its production, for example food and beverage industries, the system is capable of delivering both CO₂ of high quality as well as electricity. Skid-mounted CO₂-capture units have been delivered down to a size of 6 t per day [23], which is comparable to three units of the size investigated in this study, or roughly 1.1 MW electric power. If there is no use for the produced CO₂ it is questionable whether this is the right application for CO₂-capture.

9. Conclusion

An optimisation of a SOFC/GT system with and without CO_2 -capture has been performed using a GA optimiser. The optimiser found reasonable solutions, but also showed some difficulties using a combination of constraints and search intervals. It is believed that the implicit calculation of the stack maximum temperature in this case presents a difficult optimisation problem for the GA optimiser. It has been shown that apart from stack temperature, it is of great importance to reduce the air flow and avoid supplementary firing unless it is necessary for combustion stability. It is also beneficial to have a high degree of external reforming. Electric efficiency close to 65% has been achieved using an uncooled generic gas turbine and two SOFC stacks of 7500 cells each.

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