

# A methodology for Thermo-Economic Modeling and Optimization of Solid Oxide Fuel Cell Systems

F.Palazzi\*, N.Autissier, F.Marechal, D.Favrat,

*Ecole Polytechnique Fédérale de Lausanne (EPFL)  
Laboratory for Industrial Energy Systems  
CH-1015 Lausanne, Switzerland*

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## Abstract

In the context of stationary power generation, fuel cell-based systems are being foreseen as a valuable alternative to thermodynamic cycle-based power plants, especially in small scale applications. As the technology is not yet established, many aspects of fuel cell development are currently investigated worldwide. Part of the research focuses on integrating the fuel cell in a system that is both efficient and economically attractive. To address this problem, we present in this paper a thermo-economic optimization method that systematically generates the most attractive configurations of an integrated system. In the developed methodology, the energy flows are computed using conventional process simulation software. The system is integrated using the pinch based methods that rely on optimization techniques. This defines the minimum of energy required and sets the basis to design the ideal heat exchanger network. A thermo-economic method is then used to compute the integrated system performances, sizes and costs. This allows performing the optimization of the system with regard to two objectives: minimize the specific cost and maximize the efficiency. A solid oxide fuel cell (SOFC) system of 50kW integrating a planar SOFC is modeled and optimized leading to designs with efficiencies ranging from 34% to 44%. The multi-objective optimization strategy identifies interesting system configurations and their performance for the developed SOFC system model.

The methods proves to be an attractive tool to be used both as an advanced analysis method and as support to decision makers when designing new systems.

*Key words:* SOFC, system design, multi-objective optimization, fuel cell

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\* Corresponding author.

*Email address:* Francesca.Palazzi@epfl.ch (F.Palazzi).

## 1 Introduction

In the field of energy conversion, the optimal system design is a key issue to valorize the potential of a technology by integrating it in an optimal manner into a system. This valorization is done by defining the most appropriate system configuration and its corresponding operating conditions. By the emergence of new technologies (fuel cell, oxygen separation membrane), new concepts (co or trigeneration, hydrogen economy) and new fuels (biomass), the integrated system design becomes a critical issue for tackling the problem of sustainable development.

The importance of taking into account aspects of system optimization when designing fuel cell-based power plants had already be stressed out by Kraus (1994), that suggested several design alternatives based on the simplification of existing designs, proper mathematical optimization techniques where however not used. Fuel cell system control and design has received increasing attention throughout the years considering as well energetic and economic aspects and using sensitivity analyses (Costamagna et al., 2001) (Chan et al., 2002) (Xue and Dong, 1998) (Wallmark and Alvfors, 2002) (Hanke et al., 2005) as well as more recently optimization methods (Baratto and Diwekar, 2005) (Entchev, 2003) (Oyarzabal et al., 2004). The combination of solid oxide fuel cells with gas turbines is also increasingly considered (Lundberg et al., 2003) (Magistri et al., 2002).

In this paper, we address the problem of solid oxide fuel cell-based power plant design. Section 2 presents a systematic methodology for the design of integrated energy systems, based on thermo-economic optimization. Section 3 gives an application of the methodology to design a 50kW Solid Oxide Fuel Cell (SOFC) system. Section 4 gives the results on the application case and discusses the major outcomes. Conclusions are given in section 5.

## 2 Process design through thermo-economic optimization

Based on the use of process simulation, the simplest approach to solve process design problems is to generate and compare different configurations of the system. Generally, simulation scenarios are defined to study the sensitivity of important parameters. With the increasing complexity of energy systems, the systematic application of such methods is no longer desirable. More advanced computer aided methods are therefore being developed.

In the field of process design, a combination of process simulation, process integration and mathematical programming techniques is usually applied to

circumvent the above mentioned limitations. Many books and reviews are dedicated to such process design methods (Nishida N., 1981; Cano-Ruiz and McRae, 1998; Biegler and Grossmann, 2004; Grossmann and Biegler, 2004; Biegler et al., 1997) and most of these lead to solving optimization problems. Due to the combinatorial, non linear and discontinuous nature of the problem, the way these techniques and methods need to be combined still remains an issue. The Industrial Energy Systems Laboratory (LENI) in the Ecole Polytechnique Fédérale de Lausanne (EPFL) has developed its experience in the field of energy system design. New methods have been gradually developed and successfully applied in several research projects throughout the last ten years. Ranging from holistic urban system design (Weber et al., 2005), to advanced power plants design (Li et al., 2004; Bolliger, 2004), wood to biomass conversion (Gassner and Marechal, 2006), and fuel cell systems design (Marechal et al., 2005; Autissier et al., 2005; Palazzi et al., 2005).

The methods for the design and optimization of integrated energy systems developed in the laboratory are continuously embedded in the computer aided framework OSMOSE. The framework makes use of multi-objective optimization methods for decision making on energy system design. The purpose of the method is to help process engineers to identify and characterize design solutions for a system where the configurations are unknown *a priori*. This identification proceeds along two main steps: (1) the modeling of the system and (2) a multi-objective optimization procedure. This leads to the identification of the best configurations, which have to be further analyzed to lead up to the final design of the system.

The following paragraphs explain the proposed modeling approach and multi-objective optimization strategy.

### *2.1 Modeling strategy*

For process design, system models often include the thermodynamic and chemical description of the phenomena occurring in the steps of the process as well as the pricing of each of the equipment required for each operation. A model, therefore, involves a number of state variables describing the physical state of the system as well as its cost and its economic performances. These variables are divided into two categories: the degrees of freedom, or decision variables, which are determined by the user; and the unknowns, or dependent variables, which are computed by solving the model equations once the value of the decision variables is fixed.

We present below a systematic way to develop thermo-economic models of energy systems by assembling all the necessary equations in a structured way.

The modeling includes the definition of a superstructure as well as the separation of the performance model in different categories.

### 2.1.1 Superstructure definition

For an operation in the system, several alternative technological options are often available. The model is therefore built as a superstructure (see fig. 1) in order to include each possible configuration.

The system superstructure is built using the following procedure:

- Define the **process steps**: a process step constitutes an elementary operation that transforms the chemical species
- For each process step define the **list of options** that are going to be considered: these are based on the available technologies for the given step
- For each option establish a **performance model** describing the state and cost of the system
- Assemble the sub-models in a superstructure. The models are connected by the input and output material flows.

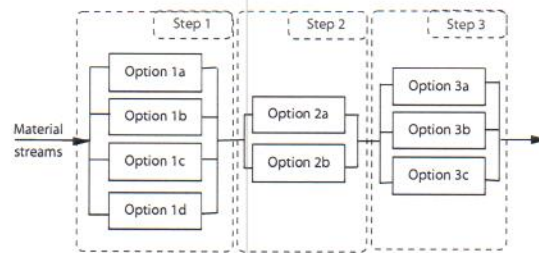


Fig. 1. Superstructure model

Once the superstructure is defined, the system consists of all the combinatorial possibilities given by the grid. However the modeling can also include constraints to prevent impossible configurations. The activation of a precise configuration will depend on the decision variables imposed.

### 2.1.2 Modeling steps

The superstructure model is solved in three successive steps: (1) the energy flow resolution, (2) the integrated heat exchange system evaluation and (3) the thermo-economic performance evaluation (see fig. 2).

- (1) The **energy flow** model computes the thermodynamic performances of the chemical and energy conversion in the superstructure. This defines the corresponding energy requirements as a function of the decision variables.

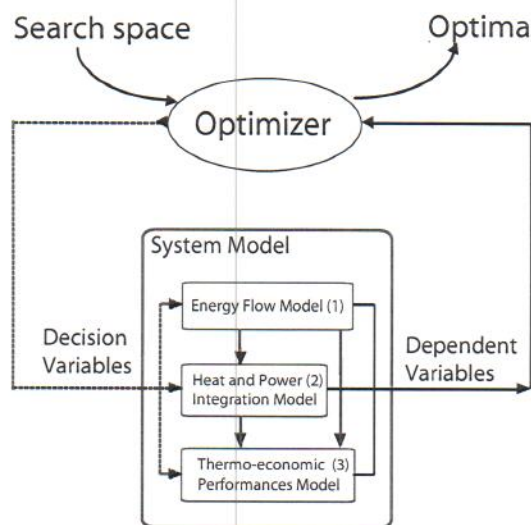


Fig. 2. Schema of the optimization procedure

For this step a commercial process modeling software is used (BELSIM-VALI), which uses an equation solver procedure.

- (2) The **heat and power integration** model is an optimization model that maximizes the combined production of heat and power. Under the assumption of the minimum approach temperature difference, the energy balance is solved under the heat cascade constraints. This model is defined using the Effect Modelling and Optimization concept presented by Marechal and Kalitventzeff (1998) and implemented in the EASY software under development at LENI. In other words, this model computes the heat exchanger network performances without having to define a priori the heat exchanger network into the superstructure.
- (3) Using the results of the energy flow and the heat and power integration models, the size of the major equipments in the system is computed, which determines the cost of the system. This is done using conventional but simplified chemical engineering methods. The costing is based on the cost estimation method of Guthrie (1969). The cost relates to the size of the equipment and the physical properties of the system by comparing it with known equipments. In the computer platform, **sizing and costing** procedures are defined as equipment modules, which can be shared by several elements of the superstructure.

Once the model is developed, it can be used to study a particular system configuration by performing sensitivity analyses. This kind of analysis indicates the trend of the model response for the main system properties under the perturbation of one or two decision variables. The other decision variables being constant. However, the observation of the system response to the variation of three or more decision variables is limited by the visualization of the results and by the number of computations to be performed. An optimization method

is therefore used to identify the most attractive configurations.

## *2.2 Multi-objective optimization strategy*

Several objectives can be formulated for defining "optimal" designs of energy systems. They are mainly of thermodynamic nature (maximization of energy efficiency, exergy efficiency), economic nature (minimization of investment cost, maximization of profits) and of environmental protection nature (minimization of CO<sub>2</sub>-NO<sub>x</sub> emissions, noise, life cycle impact). We focus here on thermo-economic optimization that considers two objectives: the maximization of system efficiency and the minimization of specific investment cost. These constitute competing objectives that indicate the performance and economic viability of a plant. These will later permit the assessment of a design in different economic contexts.

The search space of the optimization is defined by the decision variables and their bounds. These are selected by the engineer to reflect the choice on design parameters, and are given as an input to the optimizer (see figure 2). In the case of two-objective optimization, the resulting output will be a group of points, the so called Pareto curve, that represents the optimal trade-off between the two objectives.

The decision variables are separated into continuous variables that represent thermodynamic performances to be reached by the process operations, (i.e. temperature, flows, pressure or ratios) and integer variables representing the use of a technology or an interconnection in the superstructure. The optimization problem is therefore combinatorial, and by definition multimodal. From the process engineering perspective, the identification of the global optimum and the local optima can be of interest, identifying the best working zones and design alternatives. This is the reason why heuristics are sometimes used to generate optimization scenarios.

In our case, the methodology is based on the use of an Evolutionary Algorithm: MOO (Multi-Objective Optimizer) developed at LENI (Leyland, 2002), (Molyneaux, 2002). After an initialization phase that explores the search space, the algorithm uses clustering techniques to search sub-spaces with similar characteristics. From the engineering perspective, the clustering techniques allows to systematically consider different competing solutions that define local optima of the system. For each cluster of solutions, the multi-objective strategy helps defining the sensitivity of the decision variables in the optimal solution domain. Each solution can be compared to its neighbors, for example one can determine the price to pay to increase the system efficiency.

In previous work, the methodology described above has been applied to study

PEMFC systems (Marechal et al., 2005). The results constitute a superstructure model of the possible fuel cell configurations. In this paper a new superstructure model is presented for studying SOFC systems.

### 3 Solid oxide fuel cell system model description

To design a fuel cell based power plant, a SOFC system model has been established. The model is subdivided into three sub systems (see Figure 3) : fuel processing, fuel cell and post combustion. Each subsystem is modeled by the energy flow, the heat exchanger model and the thermo-economic performances model. The heat exchanger network is determined on the whole system by minimizing the exergy losses.

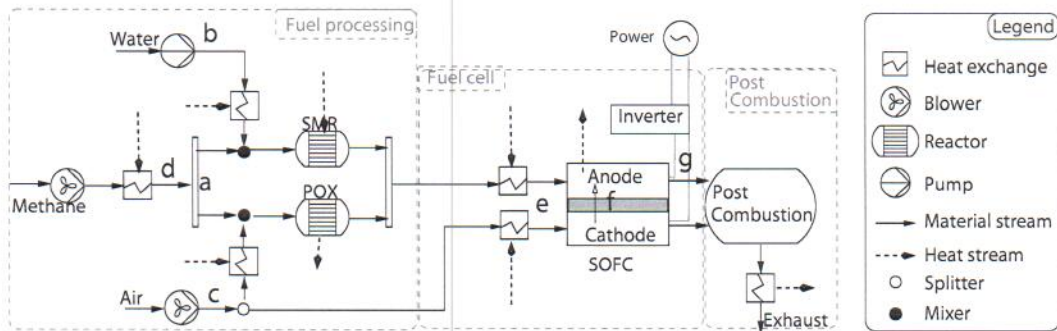


Fig. 3. Solid oxide fuel cell system model

#### 3.1 Fuel processing model

The following options are available for processing the entering natural gas: steam methane reforming (SMR), methane partial oxidation (POX) or a combination of both (see Table 1). The partial oxidation reaction is modeled by a tree reaction mechanism including complete oxygen consumption by methane combustion, equilibrium steam methane reforming and equilibrium water gas shift. The blowers and pumps are electrically driven using the power generated by the fuel cell. The sizing and costing of the fuel processing is described in (Marechal et al., 2005).

### *3.2 Solid oxide fuel cell subsystem model*

The SOFC model is based on the model developed by Van herle et al. (2003) The fuel cell features planar technology, anode supported cells, composite LSM/YSZ cathode metallic interconnects and thin electrolyte. Multiple stacks of 100 cells are supposed, with a cell area of  $200\text{cm}^2$ .

The chemical reactions considered at the anode are the complete consumption of oxygen by combustion of hydrogen and carbon monoxide as well as methane reforming and water gas shift at equilibrium (see Table 1).

The electro-chemical model includes diffusion losses at the anode and cathode, as well as ohmic and non-ohmic losses given by correlations from literature (Van herle et al., 2003).

The fuel cell inlet temperature is set at 1073 K. A limit of 100 K is fixed for the maximum temperature gradient across the fuel cell. This avoids cracks due to thermal gradient. If the heat generated inside the fuel cell leads to gradients higher than 100 K, energy is evacuated through a heat exchanger. This leads to two possible fuel cell configurations: adiabatic or cooled.

The costing model of the fuel cell is given in tables 2 and 3 and includes the cells cost, the housing cost for each stack and the cost of the housing volume that is derived from (Turton, 1998).

### *3.3 Post combustion model*

At the exit of the fuel cell, the outlet streams are mixed for post combustion of the depleted fuel in an adiabatic combustion chamber. Total combustion of the remaining fuel is supposed. Heat is recovered from the combustion gases before releasing them to the exhaust at a temperature of 100 C. This temperature may even be lowered when domestic combined heat and power at low temperature is considered.

### *3.4 Heat exchanger network optimization model*

The heat and power integration model considers cooling water as a cold utility and allows the burning of additional methane in the post combustion chamber as hot utility to close the system balance. Heat exchange is assumed with a minimum temperature difference of 60 K.



Table 1  
Chemical reactions considered in the fuel cell system model

Name	Reaction	Reaction enthalpy
Steam Methane Reforming (SMR)	$CH_4 + H_2O \Leftrightarrow CO + 3H_2$	$\Delta H_0 = 206.11kJ/mol$
Water gas shift (WGS)	$CO + H_2O \Leftrightarrow CO_2 + H_2$	$\Delta H_0 = -41.160kJ/mol$
Hydrogen combustion	$2H_2 + O_2 \Rightarrow 2H_2O$	$\Delta H_0 = -571.6kJ/mol$
Carbon monoxide combustion	$2CO + O_2 \Rightarrow 2CO_2$	$\Delta H_0 = -565.8kJ/mol$
Methane combustion	$CH_4 + 2O_2 \Rightarrow 2H_2O + CO_2$	$\Delta H_0 =$
Methane partial oxidation (POX)	$CH_4 + \frac{1}{2}O_2 \Rightarrow CO + 2H_2$	$\Delta H_0 = -35.715kJ/mol$

Table 2  
Solid oxide fuel cell model

Costing model	
Cell cost	$C_{cell} = A_{cell} \cdot C_{fc,spec}$
Number of stacks	$N_{stack} = \left\lceil \frac{N_{cells}}{N_{cells}^{max}} \right\rceil$
Housing volume cost	$C_V = 10^{K_1 + K_2 \cdot \log(\dot{Q}_{fc})} \cdot f_{BM}$
Fuel cell stacks cost	$C_{stacks} = f_{BM} \cdot (C_{cell} \cdot N_{cells} + 2 \cdot N_{stack} \cdot A_{cell} \cdot C_{h,spec})$
Housed fuel cell cost	$C_{fc} = f_a \cdot (C_V + C_{stacks})$

Table 3  
Fuel cell costing constants

Name	Value	Unit
$C_{fc,spec}$	0.1442	$\$/cm^2$
$C_{h,spec}$	0.46425	$\$/cm^2$
$f_{BM}$	2.7	-
$K_1$	2.5689	-
$K_2$	0.8067	-

## 4 Results

The model described above has been optimized to design a 50kW system. The optimization considers two objectives: minimization of the installed cost and maximization of the efficiency (see Table 5). The efficiency is computed on the lower heating value of the entering fuel. The installed cost includes the cost of the fuel cell, heat exchangers, pump and blowers, post combustion chamber and fuel reformer. The cost of piping, control and transformer are not included. The decision variables used in the search are given in Table 4, along with the constant parameters of the system.

Table 4  
Decision variables and constants for the optimization

Name	Value	Unit
DecisionVariables		
$T_{reformer}$	[800 ; 1073]	K
$\mu$	[0.5 ; 0.9]	-
$\xi_{OC}$	[0.001; 0.5]	-
$\xi_{SC}$	[0.4 ; 4]	-
$\lambda$	[1.5 ; 5]	-
Constants		
Delivered power	50	kW
Inverter efficiency	0.9	-
$i$	4000	$A/cm^2$
$T_{exhaust}$	373	K
$A_{cell}$	200	$cm^2$
$T_{FC}$	1073	K

Table 5  
Objectives of the optimization problem

Objectives	
System efficiency	$\epsilon = \frac{\dot{E}_t - \dot{W}_{res}}{LHV_{fl,in} \cdot \dot{n}_{fl,in}}$
System installed cost	$C_{syst} = C_{fc} + C_{htx} + C_{fp} + C_{pc} + C_{pb}$

The Pareto curve on Figure 4 represents the results of the optimization with clusters of optimal points in the objective space. The optimizer identifies four clusters of solutions  $a, b, c, d$ . The configurations belonging to cluster  $a$  have relative low costs of 158'700\$ to 161'900\$ with efficiencies ranging from 0.297 to 0.345. Cluster  $b$  solutions display efficiencies from 0.376 to 0.425, with the corresponding costs from 162'500\$ to 207'800\$. Cluster  $c$  solutions present high efficiencies, from 0.425 to 0.439, the costs range from 212'800\$ to 277'700\$. Cluster  $d$  solutions are slightly in the Pareto sub-optimal space with prices of 171'500\$ for 0.331 efficiency to 269'600\$ for 0.430 efficiency.

For the decision maker, these results are a first indication on the design selection. Considering the available capital, the most efficient design is identified on the Pareto curve. Also, the decision maker might consider to increase its investment when the effect on the efficiency is high, as in the lower part of the Pareto, where an increase of 2% on the investment cost leads to 16% higher efficiency. On the other hand, increasing the investment cost is less attractive

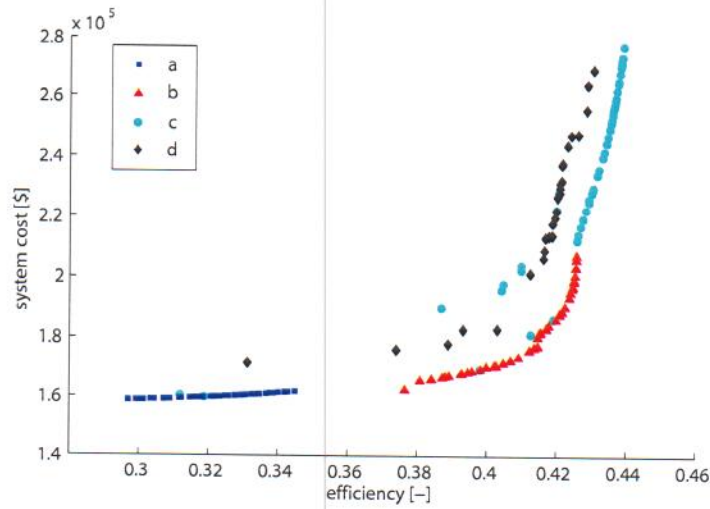


Fig. 4. Optimal points

in the upper part of the Pareto, as an increase of 30% in the investment, leads only to a 3% higher efficiency.

From the engineer perspective, the detailed analysis of the Pareto optimal configurations provide also indications on the system behavior as well as trends for R&D strategies. Figures 9, 7, 11, 5, 6 show the projection on the efficiency axis of the value of the decision variables (Table 4) corresponding to the optimal solutions.

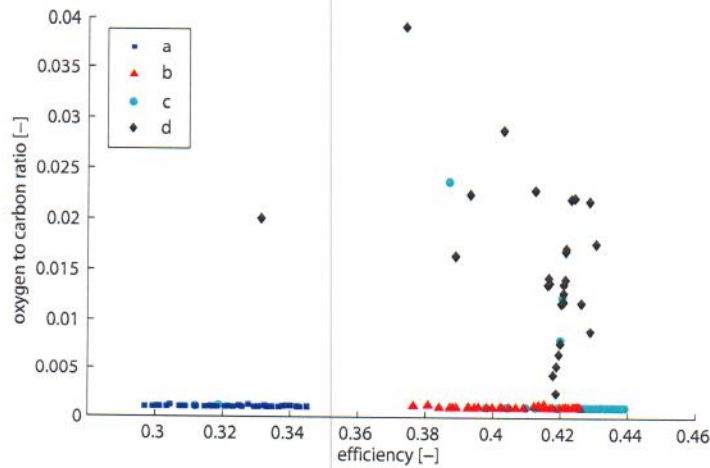


Fig. 5. Oxygen to carbon ratio of the optimal points

The steam to carbon ( $\xi_{SC}$ ) and the oxygen to carbon ( $\xi_{OC}$ ) ratio hit their lower bounds for all the solutions, except in cluster *d* that is suboptimal, indicating a preference for internal reforming in all the designs. This is explained by the fact

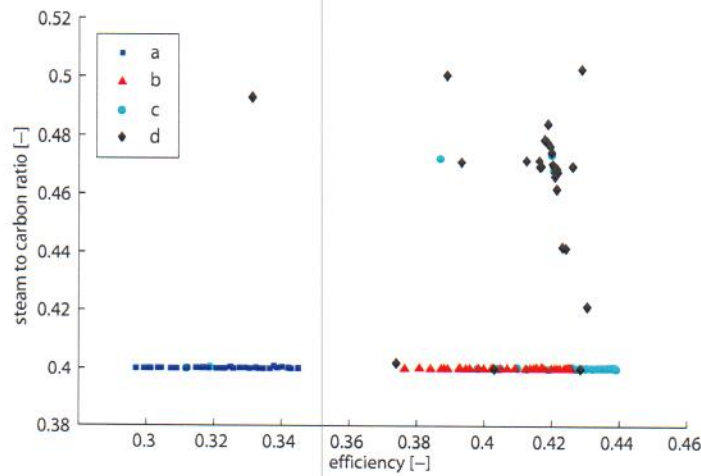


Fig. 6. Steam to carbon ratio of the optimal points

that internal reforming does not imply heat exchange between the reformer and the fuel cell. Therefore, there is no heat degradation due to external heat exchange. These solutions however would require to have a suitable catalyst in the fuel cell that allows the internal reforming.

Figure 7 shows that the less expensive action to increase efficiency is to design fuel cells with higher fuel utilization ( $\mu$ ). This has the effect of increasing the fuel cell cost as depicted in Figure 8. When fuel utilization reaches its higher bound, 0.9 for a 42.5% efficient system, other means have to be found to further increase efficiency.

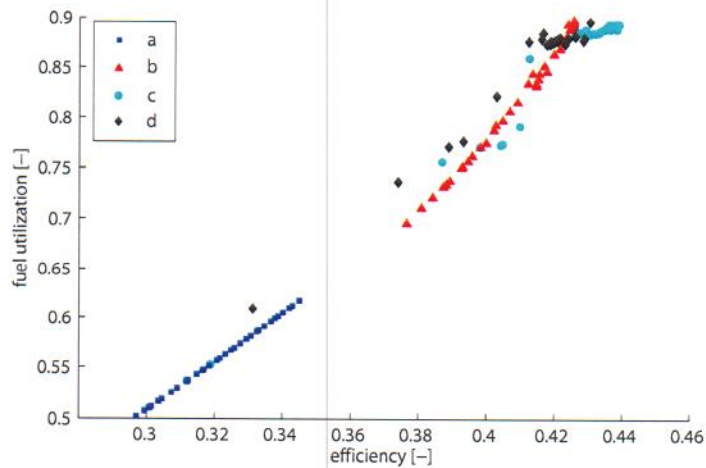


Fig. 7. Fuel utilization of the optimal points

The fuel processing temperature (Figure 9) is at its maximal bound (1073 K) for all the Pareto-optimal systems below 42.5% efficiency (clusters *a* and *b*).

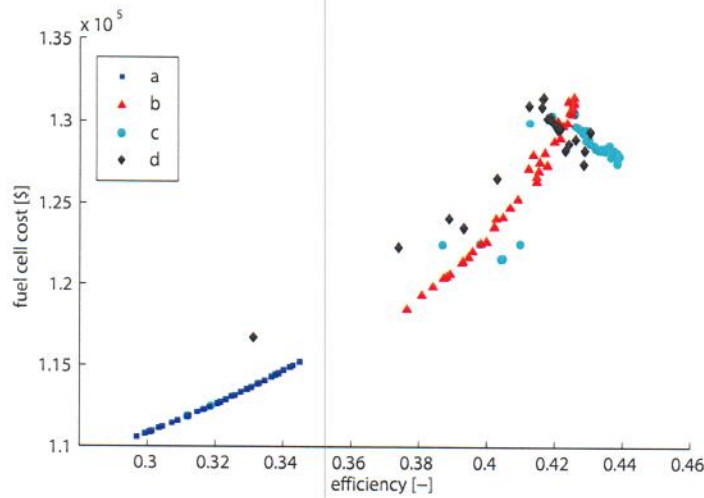


Fig. 8. Cost of fuel cell of the optimal points

Cluster *c* shows that, as the fuel utilization is maximal, there is an interest in decreasing the temperature to achieve higher efficiencies. This, however, will increase the cost of the system, as the volume of the reformer increases to convert all the entering steam (Figure 10).

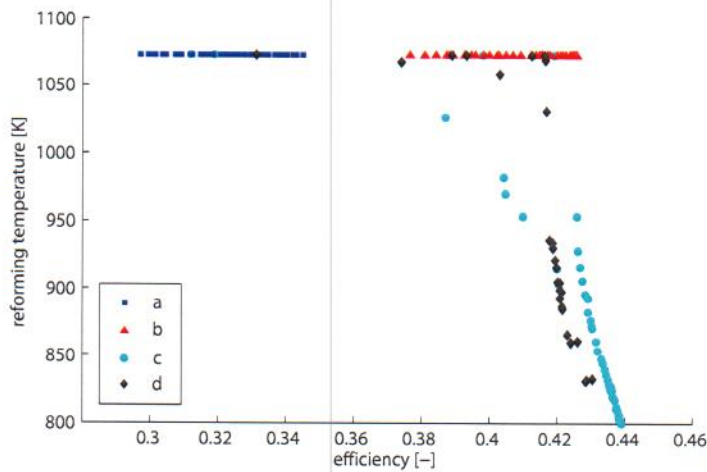


Fig. 9. Fuel processing temperature of the optimal points

Figure 11 displays the air excess ratio ( $\lambda$ ) variation along the Pareto curve. Cluster *a* solutions with lower efficiency and lower cost are distinguished by their air excess ratio hitting the lower bound. Cluster *b, c* and *d* have air excess ratio values between 2 and 4.

The number of cells of each configuration is shown in Figure 12, with the corresponding number of stacks. As the current density is constant, the cell potential exhibits a reverse pattern 13.

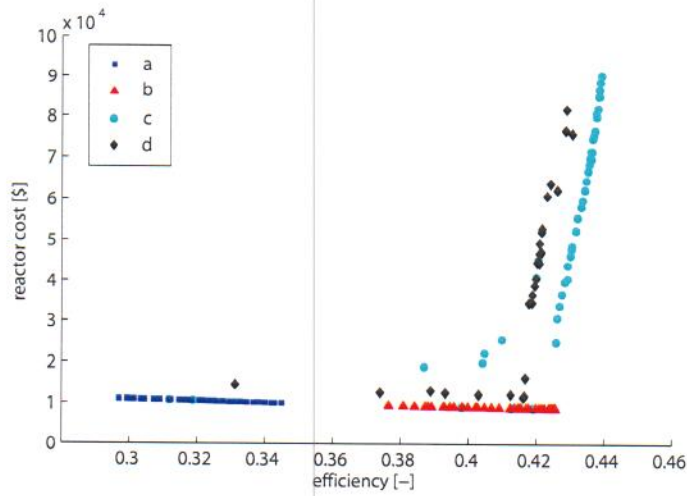


Fig. 10. Cost of fuel reformer of the optimal points

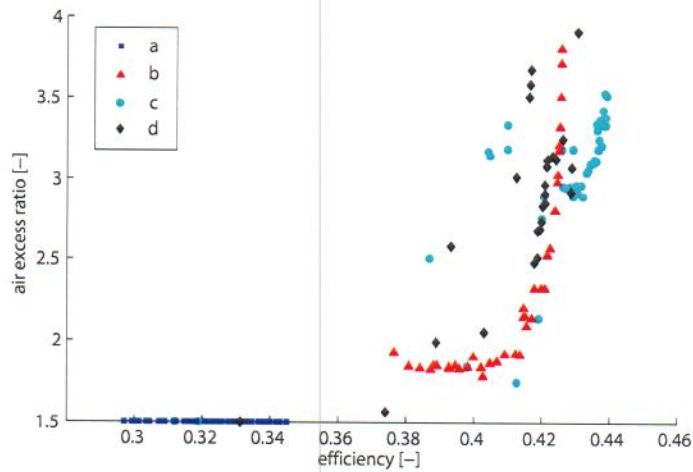


Fig. 11. Air excess ratio of the optimal points

The heat integration of all systems do not present a pinch point. Additional firing is therefore never required. Hence the systems are globally exothermal with the excess heat evacuated by cooling water. The excess of heat shows the possibility of integrating combined heat and power devices like organic or steam Rankine Cycles. The composite curves of the least an most efficient points of cluster a (Figure 14) show the main heat exchanges appearing in the system. The hot streams are: the fumes cooling (A,C), and the heat evacuated from the stacks (B). This heat is exchanged with the cold streams, preheating before the fuel reforming (E), and before the fuel cell (F), and the cooling water (D). The increase in fuel utilization from the left to the right figure increases the heat evacuated from the fuel cell and decreases the temperature of the post combustion outlet, decreasing the distance between the hot and the cold composites and thus the need for cooling water.

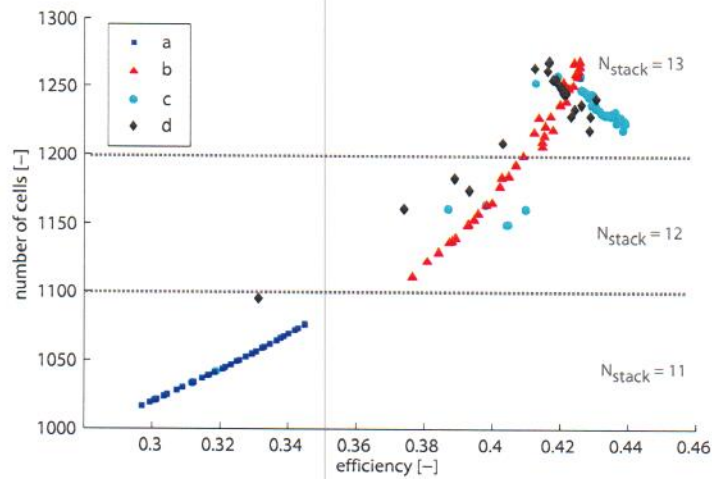


Fig. 12. Number of cells of the optimal points

The same happens as the fuel utilization increases from the least efficient to the most efficient point of *b* (Figure 15).

In cluster *c*, the decrease of the fuel processing temperature implies that the content of methane at the fuel cell inlet is higher, therefore there is more internal reforming and less heat to removed from the fuel cell by heat exchange in order to maintain a heat gradient of 100K along the cells (Figure 17). With practically constant post combustion temperature, the composite curves of cluster *c* get closer as the heat evacuated from the fuel cell decreases, leading to higher global efficiencies.

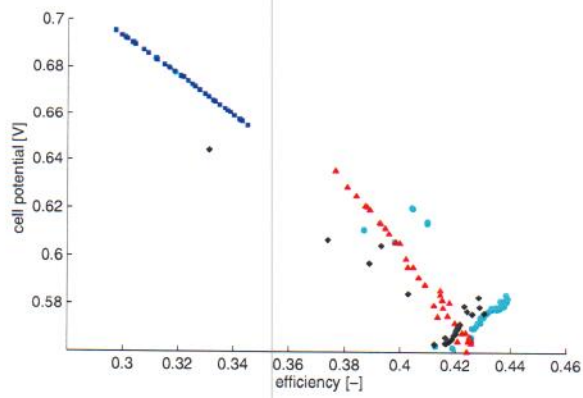


Fig. 13. Cell potential of the optimal points

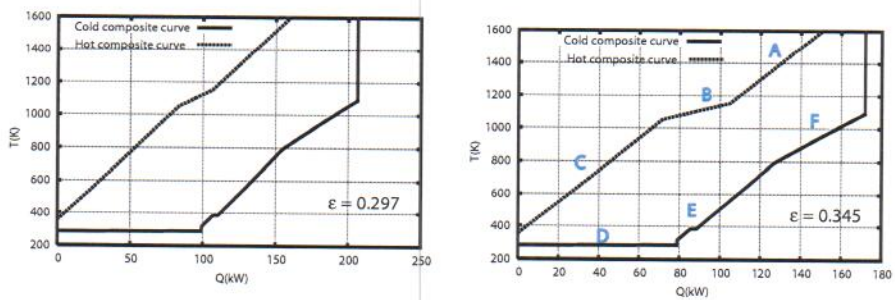


Fig. 14. Composites curves of the extreme points of cluster a



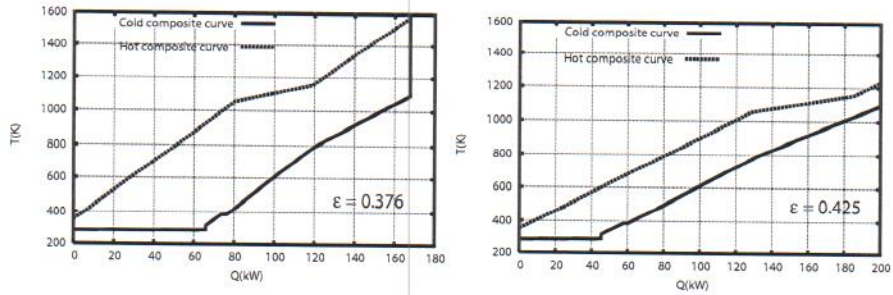


Fig. 15. Composites curves of the extreme points of cluster *b*

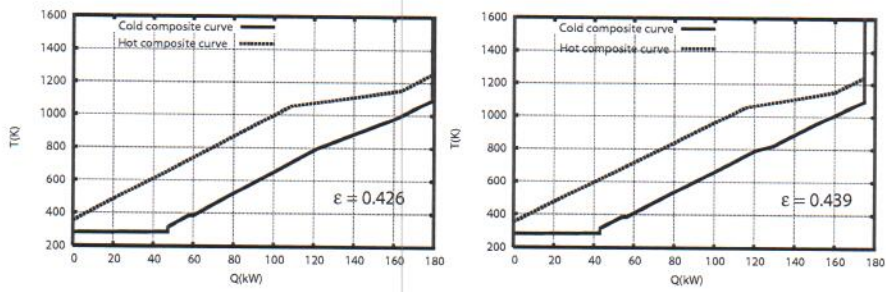


Fig. 16. Composites curves of the extreme points of cluster *c*

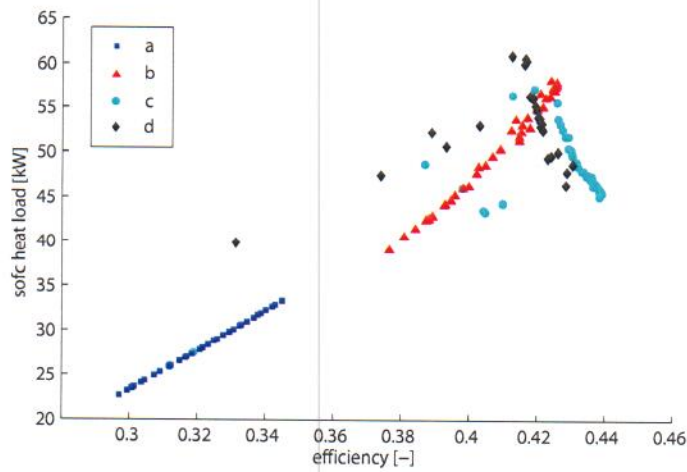


Fig. 17. Heat to be exchanged in the fuel cell for the optimal points

## 5 Conclusions

The proposed energy system design methodology has been applied to design a 50 kW system. This method combines thermo-economic modeling, heat integration and multi-objective optimization in a modular way. As it has been noticed, the results of the thermo-economic optimization offer a base for decision making and discussion. The trade-off curve can be used to select a design according to available capital. Moreover, the systematic analysis of the computation results deepens the understanding of the impact of design decisions on the system operating conditions. From this analysis, design improvements can emerge that were not foreseen in a first step.

The considered fuel cell systems all present an excess of heat at high temperature. This indicates that new subsystems realising the heat to electricity conversion have to be integrated for a better valorization of the high temperature fuel conversion. Gas turbines hybrid cycles that combine a gas turbine and a solid oxide fuel cell are a good candidate to further use the heat generated by the fuel cell. The modularity of the modeling strategy allows the rapid integration of these improvements for a successive analysis, as addressed by the authors in (Autissier et al., 2005). For smaller size systems, the integration of Rankine cycles would be a viable option.

## 6 Acknowledgment

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## 7 Nomenclature

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$A_{cell}$	Cell area [ $cm^2$ ]
$C_{cell}$	Cost of one cell [\$]
$C_{fc,spec}$	Specific cost of a cell [ $\frac{\$}{cm^2}$ ]
$C_{fc}$	Fuel cells total cost [\$]
$C_{h,spec}$	Specific cost of stack housing [ $\frac{\$}{cm^2}$ ]
$C_{htx}$	Heat exchangers cost [\$]
$C_{pb}$	Pump and blowers cost [\$]
$C_{pc}$	Post combustion chamber cost [\$]
$C_{stacks}$	Stacks cost [\$]
$C_{syst}$	System cost [\$]
$C_V$	Stacks housing volume cost [\$]
$\dot{E}_t^-$	Electricity produced at the transformer output [kW]
$f_a$	Actualization factor
$f_{BM}$	Bare module factor
$i$	Cell current density [ $A/cm^2$ ]
$K_1, K_2$	Constants for housing volume cost computation
$LHV_{fl,in}$	Lower heating value of the entering fuel [ $kJ/kmol$ ]
$\dot{n}_{fl,in}$	Entering fuel flowrate [ $kmol/s$ ]
$N_{stack}$	Number of stacks
$N_{cells}^{max}$	Maximal number of cells in a stack
$N_{cells}$	Number of cells
$\dot{Q}_{fc}$	Fuel cell housing thermal load [ $kW$ ]
$T_{reformer}$	Temperature of the reformer [ $K$ ]
$T_{exhaust}$	Temperature of the exhaust gases [ $K$ ]
$T_{FC}$	Operating temperature of the fuel cell [ $K$ ]
$\dot{W}_{res}$	Electrical power required by auxiliaries [ $kW$ ]
$\mu$	Fuel utilisation in the fuel cell [-]
$\xi_{OC}$	Oxygen to carbon ratio [-]
$\xi_{SC}$	Steam to carbon [-]
$\lambda$	Air excess[-]

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