

## MAN-PORTABLE POWER GENERATION BASED ON FUEL-CELL SYSTEMS

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### Abstract

Micro-fabricated fuel cell systems are a potential consumer product with the promise to out-perform batteries for man-portable power generation in terms of the achievable energy density. A great variety of potential devices are being considered in various research institutions and thus there is a need for a systematic product design methodology, including comparison of alternatives and examination of the influence of technological parameters. The design of these product/process hybrids is inherently different from macro-scale process design because of the differing design specifications, objectives and constraints, as well as the relative importance of the underlying physico-chemical phenomena. The influence of heat losses is such that flowsheet design and layout need to be considered simultaneously. We have developed a methodology for the comparison of alternatives; we consider a variety of fuel/chemical choices, including hydrocarbons, methanol, ammonia and hydrides, as well as options for oxygen supply; fuel cells types considered are Solid Oxide Fuel Cells, hydrogen operated Polymer Electrolyte Membrane Fuel Cells, Direct Methanol Fuel Cells, Proton Ceramic Fuel Cells and Single Chamber Fuel Cells. In this paper we present our methodology and a case study, showing the effect of layout options and fuel combinations.

# 1 Introduction

The ever-increasing use of portable electric and electronic devices increases the need for efficient autonomous man-portable power supplies [1, 2]. Currently, batteries are the predominant technology in most applications. However, batteries have a large environmental impact, high cost and relatively low gravimetric (Wh/kg) and volumetric (Wh/l) energy densities. State-of-the-art primary batteries reach up to 1300 Wh/l and 700 Wh/kg and rechargeable up to 400 Wh/l and 300 Wh/kg [3, 4]. The upper limit on battery performance is now being reached as most of the materials that are practical for use as active materials in batteries have already been investigated and the list of unexplored materials is being depleted [2, 3].

There are two main approaches for fuel cell systems, namely direct fuel cells running on stored hydrogen, methanol, formic acid, or medium sized hydrocarbons, as well as fuel processing for hydrogen or syngas generation and subsequent oxidation of these intermediates in a fuel cell. Micro power generation devices based on either approach are products that comprise a more or less complex chemical process. There is a plethora of possible processes and process combinations, as well as a wide variety of applications and consumers, ranging from cellular phones and laptops for home use to the power needs of the dismounted soldier, thus it is plausible that the optimal device configuration will depend on the product specifications characterizing particular applications. This necessitates a flexible methodology for the comparison of different technology alternatives that can facilitate product engineering of these devices.

In macro-scale processes design is performed in stages, e.g., [5, 6], and plant layout is typically addressed independently of and subsequently to the design of the flowsheet. At the micro-scale the process components are highly integrated and heat losses significantly influence the process performance [7] and possibly the optimal design, so that the problems of flowsheet design, physical layout and integration of heat sinks and heat sources need to be addressed simultaneously. A very promising approach is to couple two or more unit operations thermally in a near-isothermal stack [8].

## Methodology

Most power consuming devices are not operated constantly and have rapidly changing power demands, and therefore the dynamics and operation of power generation devices are very important. Similar to the electric vehicle application [9], a fast start-up procedure, at most on the order of minutes, is required. In this paper we consider the steady-state performance under the assumption that the devices will be able to respond to power demands rapidly and therefore the average performance will most likely be dominated by the steady-state behavior of the devices. For the calculation of energy density, we include the mass/volume of the device, an auxiliary battery as well as the fuel cartridge for a given mission duration (time between refueling).

As possible fuel/chemicals we consider hydrocarbons, methanol, ammonia and hydrides; for the oxygen supply we consider atmospheric air, compressed air, compressed oxygen and oxygen generators; fuel cells types considered are Solid Oxide Fuel Cells, hydrogen operated Polymer Electrolyte Membrane Fuel Cells, Direct Methanol Fuel Cells, Proton Ceramic Fuel Cells and Single Chamber Fuel Cells. The flowsheets considered were chosen with the constraint that the realization of the processes is either currently under investigation or foreseeable in the short term future (coming years).

We graphically represent the alternatives considered by a flowsheet superstructure (Figure 1). We want to emphasize that the superstructure is only conceptual, and several of the “units” can actually be physically combined and our models account for thermal integration of the processes. Our intention is to have a general methodology that can cover various geometries and reactor types (PFR, CSTR, packed bed, etc.) and be independent of the specific catalysts used and therefore our models are based on user specified efficiency parameters in the various units like conversion, electrochemical efficiency, separation efficiency, etc. Once these parameters, as well as the operating conditions have been specified, the performance of the system is calculated. The physical properties used are described in [7].

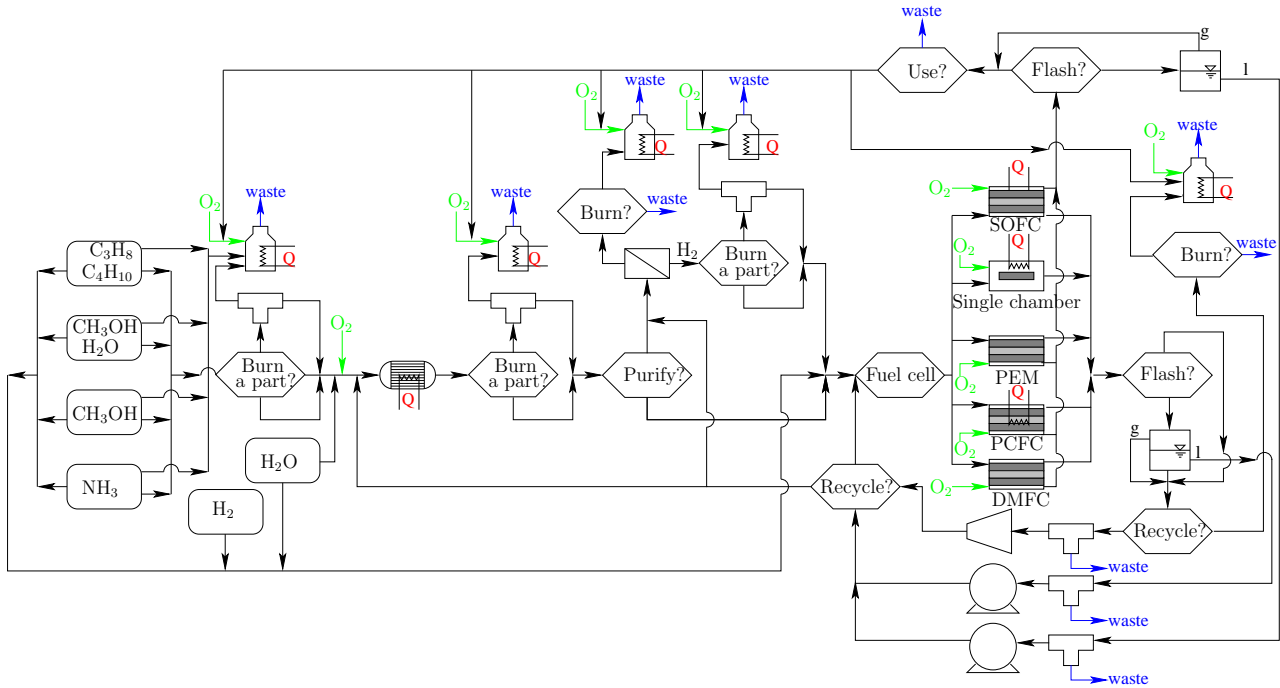


Figure 1: Conceptual process superstructure.

## Integrated Layout and Thermal Management

The graphical representation of the superstructure (Figure 1) does not contain information about the physical layout. In [7] we demonstrated the pronounced effect of heat losses on process performance and the importance of thermal management for high-temperature micro power generation devices. A very promising approach for thermal management is to couple two or more units thermally in a near-isothermal stack [10]. In this manner direct heat transfer between heat sinks and heat sources is possible, as well as heat recovery of the effluent streams; thermally coupling two units also reduces the surface area and as a consequence the heat losses. Combining units is thus a layout consideration that influences the process performance. As a consequence, the problems of flowsheet design, physical layout and heat integration need to be solved simultaneously.

We propose an idealization of the layout considerations, allowing only for two extremes. One extreme is that the units are thermally connected, so that they share the surface that results in heat losses, and one energy balance is sufficient. The other extreme that we consider is that the units are separated, so that each one has separate heat losses to the ambient and significant heat losses occur when mass or heat are transported between the units. In Figure 2 the two extreme cases of layout are illustrated for a process, in which butane is partially oxidized and the syngas produced is fed into a SOFC, while the cathode effluents are used to oxidize the unburned syngas from the anode for heat generation. In one extreme case the SOFC, reactor and burner are assumed to be thermally coupled, while in the other extreme case, all three process components are separate, with distant heat exchange between the burner and the SOFC. It should be noted that also Figure 2 is conceptual and not an actual design.

## Case Study

Within the scope of this paper it is not possible to provide a great number of case studies, but rather an example of the capability of the methodology developed. It should be noted that the numerical results depend on the values of the operating and modeling parameters used. We investigate the effect of using a second fuel for heat generation as well as how different layouts can yield significantly different system performances. A process that has been proposed, e.g. [11], is ammonia decomposition to nitrogen and hydrogen and subsequent oxidation of the hydrogen in a PEM fuel cell. A major drawback of this process is that ammonia is corrosive and extremely toxic. From a technological point of view this process has the benefit that the ammonia does not contain carbon, and thus poisoning of the PEM can be avoided without the need for a separation following the fuel processing. However, the process has many drawbacks, including high operating temperatures for the fuel processing reactor and an endothermic fuel processing reaction, so that burning the fuel cell effluents may not provide sufficient heat [7]. Performance improvements can be achieved by the use of a second high energy fuel, e.g., hydrocarbons, for

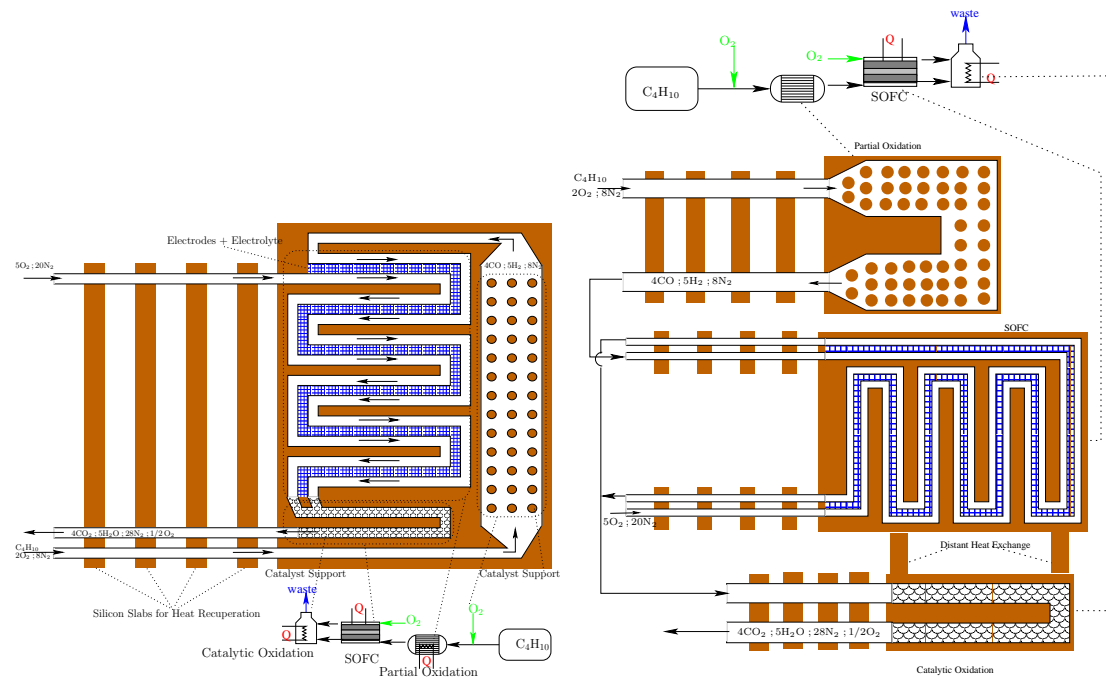


Figure 2: Conceptual difference between coupled (left) and non-coupled (right) process components.

heat generation. We consider two extreme cases of layout, namely that either the two burners are separate and we have remote heat exchange or that the two streams to be burned are combined in a burner which is in thermal contact with the reactor. In [12] it was demonstrated that the conversion for ammonia cracking reaction is essentially complete for residence times in the order of ms and a fuel processing temperature of  $650^{\circ}C$ . Here we assume complete conversion of ammonia in the reactor and vary the residence time in the reactor in the range  $0 - 100ms$ . Table 1 summarizes the parameters used and Figure 3 shows the results in terms of the fuel energy density.

Even for low residence times combining units into a stack has a significant impact, and the thermal integration seems necessary. This case study illustrates that flowsheet design and thermal management, including combination of heat sources and heat sinks need to be considered simultaneously. The use of ammonia oxidation for heat generation in separate units becomes essentially impossible for high residence times because of the resulting increase in heat losses. The choice of a single fuel or a fuel combination is not obvious; from a perspective of maximizing the energy density fuel combination is very advantageous, but it bears the logistic difficulties of carrying two fuels. This tradeoff implies that for different applications a different design will be used.

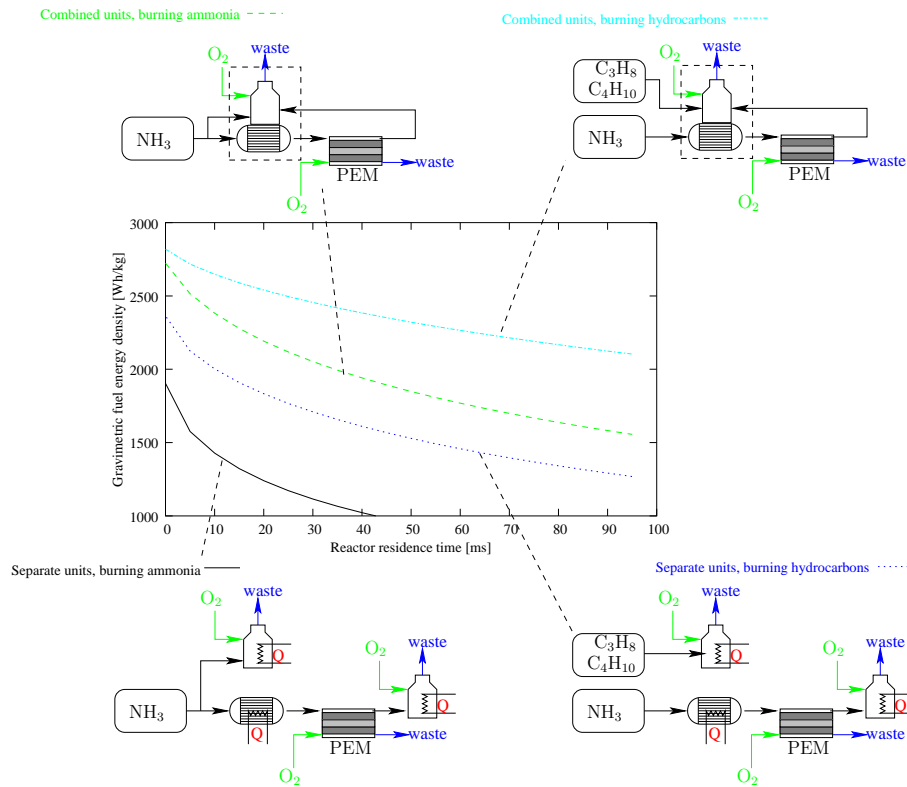


Figure 3: Effect of fuel combinations and layout options on gravimetric fuel energy density of an ammonia-cracking based process.

## Conclusion and Future Work

Micro power generation devices based on fuel cells are products with the potential of outperforming batteries for man-portable power generation by an order of magnitude in terms of energy density. There is a plethora of conceivable applications and processes and this results in the need for product engineering. We have presented a methodology for the comparison of the alternatives and investigation of the influence of technological parameters. We have implemented the methodology as a tool available in the form of a web-interface [13], which allows for facile use by remote users, who are unfamiliar with the modeling language and the details of the models. Upon request and subject to approval this web-interface can be made available for academic purposes.

At the micro-scale, process components are highly integrated and the heat losses strongly influence the optimal design, so that the problems of flowsheet design, physical layout, and integration of heat sinks and sources need to be solved simultaneously. The optimal process design depends on product specifications and technological advances. The performance of water consuming reactions depends strongly on the ability to separate and recycle the waste water.

Table 1: Process parameters for the ammonia cracking case study, Figure 3.

Ambient temperature	$T_{amb} = 298\text{K}$	Power output	$PW = 1\text{W}$
Reactor temperature	$T_{op} = 923\text{K}$	Discard temperature from reactor	$T_{out} = 623\text{K}$
Conversion in burners	$\zeta = 0.95$	PEM temperature	$T_{op} = 350\text{K}$
Residence time in burners	$\tau = 1\text{ms}$	Discard temperature from PEM	$T_{out} = 350\text{K}$
Air excess in burners	$\Phi = 1.2$	Conversion in fuel cell	$\zeta = 0.8$
Overall heat loss coefficient	$U = 3\text{W}/\text{m}^2/\text{K}$	Residence time in fuel cell	$\tau = 20\text{ms}$
Emissivity (incl. view factor)	$\epsilon = 0.2$	Efficiency of fuel cell	$\eta_{FC} = 0.7$
Air excess in fuel cell	$\Phi = 1.2$	Compression penalty in air feed	$K_C = 10\text{J}/\text{mol}/\text{K}$
Burner temperature	$T_{op} = 1000\text{K}$	Discard temperature from burner	$T_{out} = 500\text{K}$
Temperature loss factor	$\chi_{temp} = 0.6$	Heat loss factor	$\chi_{heat} = 0.6$

Our modeling framework is flexible and we are considering the inclusion of more fuels, e.g., formic acid [14] or different fuel processing mechanisms, e.g., autothermal reforming [15]. We also intend to obtain some good estimates for the size of peripheral components, such as valves and pumps, but in contrast to the macro-scale the energy consumption and influence of these components may be substantial and should be considered.

Under the assumption that rapid start-up operation is possible, the average performance mainly depends on the steady-state performance of the processes; nevertheless, the transient behavior is extremely important and needs to be addressed in detail. Also our models do not account for the kinetics and cannot predict some important process operating conditions such as fuel to air ratio required. First results to cover these two aspects are presented in [16].

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