OPTIMAL DESIGN AND OPERATION OF FUEL CELL SYSTEMS FOR MICRO POWER GENERATION

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Abstract

Currently, the predominant technologies for autonomous portable electrical power supply are batteries. A promising potential alternative is devices that generate electrical power through electrochemical conversion of easily stored fuels in microfabricated fuel cells. These devices are consumer products that are entire micro-scale chemical processes, and it is necessary to explore their optimal design and operation. A modeling framework is presented for the evaluation of design alternatives, focusing on the combination of syngas production and fuel cells, and a power production in the range 0.1-10W. Product specifications are discussed and a process superstructure, including hundreds of different designs, is formulated. Scalability issues are identified and discussed, and the influence of scale on the process performance, as well as the tradeoffs between different designs are presented in a case study.

Keywords

Man-portable power, Micro power generation, Micro fuel cell system, Product design

Introduction

The widespread use of portable electric and electronic devices increases the need for efficient autonomous man-portable electrical power supplies (up to 50 W) Jacobs et. al. (1996), Dyer (2002). 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 density and the upper limit on performance is now being reached Linden (2001), Brodd (1999).

Out of the possible alternatives we are focusing on electrical power generation processes employing electrochemical conversion of common fuels and chemicals, such as hydrocarbons or alcohols, in fuel cells. These processes have the potential to yield much higher energy densities than state-of-the-art batteries, because on one hand the afore mentioned fuels have very high energy contents, and on the other hand fuel cells can in principle achieve very high efficiencies. One approach is the use of direct fuel cells, running on methanol, formic acid or medium sized hydrocarbons, and another is fuel processing for hydrogen or syngas generation and subsequent oxidation of the hydrogen or syngas in a fuel cell.

Micro power generation devices are potential consumer products that comprise sophisticated chemical processes, and the challenge of their optimal design and operation is addressed in this paper. In order to achieve portability, the use of micro-fabricated devices, as opposed to conventional devices, is necessary. While systematic process synthesis and design is a mature field at the macro-scale, micro systems exhibit a unique set of new challenges for process systems engineering. For example, at the micro-scale heat losses to the environment are a critical design consideration. The portability requirement, as well as the fact that the devices need to work fully automatically without the intervention of operators and without any safety concern, also give rise to many design constraints and safety issues.

In larger scale power production emphasis is placed on efficient utilization of the fuel, whereas in portable power production the design objectives and constraints are inherently different. Typical evaluation metrics include specific energy [Wh/kg], volumetric energy density [Wh/l] and price. For the calculation of energy density it is necessary to include both the fuel and the device mass/volume, e.g., Dyer (2002). Ideally micro-power generation processes should be inherently safe and pose no health concern whatsoever. This requirement is probably unrealistic and can reasonably be relaxed to allow fuels and devices that pose health and safety concerns similar to chemicals used in common consumer applications.

Methodology

While batteries are a well-established product, micro power generation processes are novel products and the desired product specifications are not yet accurately known. Moreover, there is a wide spectrum of applications and consumers from cellular phones to power supply for the dismounted soldier. Batteries are usually assessed in terms of their energy density Linden (2001), Brodd (1999), as well as cost and life expectancy, and it is to be expected that a micro power generation process will only have practical applications if it is competitive to state-of-the-art primary and/or rechargeable batteries in terms of energy density and cost. Since the fabrication of these processes uses similar technology to that of electronic devices, it is likely that fabrication of the power generation process can be integrated with that of the power-consuming device. Thus, the cost of fabrication can be spread over the life cycle of an electronic device. Other important factors are the reliability of the products, their tolerance to varying ambient conditions, a minimal environmental impact, a fast response to changing power demands and a long lifetime of the devices. At this moment it is unclear what the primary objective is, and the relative importance of the above-mentioned factors largely depends on the specific application. Also the achievable performance of the reactors, fuel cells and peripheral devices is under constant improvement. Therefore any methodology or tool for the assessment of alternatives needs to be flexible in terms of the design objectives and constraints.

In order to address the challenges of product design for micro-chemical systems we are utilizing process systems engineering tools, adjusted to reflect the physical phenomena that dominate at the micro-scale and the special characteristics of these devices. In an extension of Mitsos et. al. (2004) we have postulated a superstructure of possible processes (Figure 1) combining chemical production of hydrogen or syngas with subsequent electrochemical conversion of the syngas in a fuel cell, and we have formulated preliminary models for direct micro-fabricated fuel cells. The superstructure was formulated with the constraint that the realization of the processes is either currently possible or foreseeable in the short-term future (next years).

The design choices are represented in Figure 1 with hexagons. The various units (reactor, burners, etc.) should not be interpreted in the traditional unit operation design paradigm, but rather as closely interconnected parts of an integrated process. The superstructure is only conceptual and does not include any information about the physical layout of the units. For example it is possible to combine several burners into one physical unit or utilize a reactor concept similar to the ones described in Arana et. al. (2003) that allows the connection of exothermic and endothermic reactions and heat recovery from the effluent streams.

The fuels considered so far are propane/butane mixtures, methanol and ammonia. While at the macro scale natural gas is often used for power production in fuel cell systems, for a man-portable application methane, ethane and hydrogen do not seem promising, because these components are supercritical or near critical at ambient conditions and their storage is problematic and therefore were not included in our study. We consider three options for the oxidant, namely atmospheric air, compressed air and compressed oxygen, which for simplicity are not shown in Figure 1.

At the micro scale only relatively simple processes are possible (Rinard 1998, Saha and Rinard 2000) and therefore our postulated superstructure contains only one reactor. As a first step in the optimal design we modeled the superstructure using equation-oriented simulation with our in-house software packages ABACUSS II (Tolsma 2002) and DAEPACK (Tolsma 2000). The equation-oriented simulation allows us to create flexible, customized models. For a specific design choice, operating conditions, and operating parameters, key figures are calculated, such as energy density, fuel flow rates, required process volume, and sensitivity of energy density with respect to the operating parameters. We have linked our models to a web-interface (Mitsos and Barton 2003) for the easy use of this tool by remote users, 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. We have performed extensive parametric studies comparing different alternatives and we plan to link these models to optimization solvers.

Case Study

The scalability of micro power generation devices is particularly interesting since there are two major scales. One is the nominal power output, which is associated with the device size, and the other is the time between refueling (mission duration), which is associated with the fuel cartridge size. In this subsection we present their influence on achievable system performance using volumetric energy density as the figure of merit. It should be noted that the results are only qualitative in the sense that they strongly depend on the chosen operating conditions and unit-performance parameters. In this case study we use the same set of parameters as in Mitsos et. al. (2004) with the addition of the necessary volume ratio.

The device size can be estimated by calculating the necessary volume for the units and multiplying with a factor accounting for the volume necessary for the packaging of the devices. This factor is dependent on the fabrication and packaging methods; a rough estimate is that the factor can be between 2 and 10 and we assumed a value of 10 here. Figure 2 shows the achievable energy densities in Wh/(l system) for a process based on butane partial oxidation and an SOFC as a function of the power output for different values of duration. For low power outputs the heat losses dominate over the exothermicity of the fuel processing, and burning of the fuel cell effluents as well as part of the fuel is needed. Since the heat losses and the heat generation scale differently with the power output the achievable energy density increases with the power output. At about 2.8W a kink is observed, because for higher power output the heat generation is sufficient and the process performance does not depend on scale. The energy density increases with duration and approaches the energy density with respect to the fuel volume.

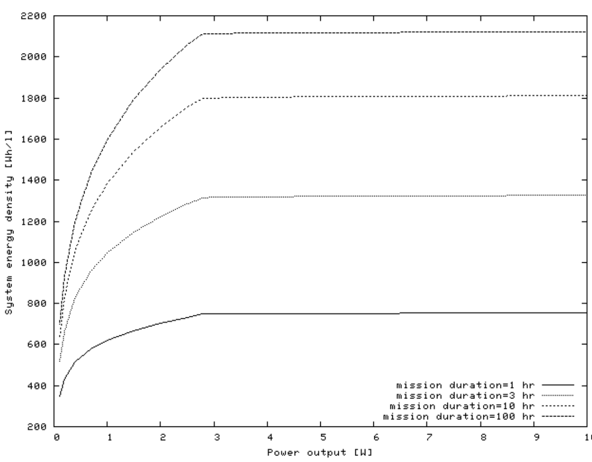

Figure2. Effect of scale on process performance

Not only the achievable performance, but also the optimal design may depend on the specified mission duration, since tradeoffs between device size and fuel volume are observed. Figure 3 compares the achievable energy density in Wh/(l system) of the butane-based process for the case that an SOFC is used with the case that gas purification and a PEM are used. While the PEM-based process achieves a higher energy density for low power outputs and duration, the SOFC-based process outperforms the PEM-based process for high power outputs or duration.

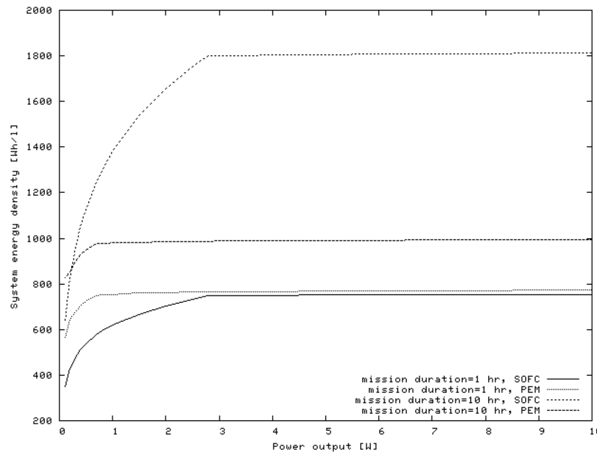

Figure 3. Effect of scale on optimal design

Conclusion and Future Work

We have applied process systems engineering tools to a problem in product engineering and created a methodology and a tool for the evaluation of different micro power generation technologies. At this moment our models include only an overall energy balance and we have not addressed the very important problem of coupling heat sinks and heat sources. This problem is more challenging than at the macro scale, and the heat exchange network synthesis (Biegler et. al. 1997) method does not seem promising, because of the increased rate of heat transfer which inevitably leads to an increased importance of heat losses. We also plan to extend the set of possible designs and specifically look into the option of combining different fuel sources, e.g., with the combination of exothermic and endothermic fuel processing reactions, as well as the on-demand generation of oxygen.

Following the paradigm of multiscale modeling we plan to apply computational fluid dynamics tools on a subset of the possible designs. This will provide a better understanding of the power and heat production as well as the temperature gradients and give insights into the problem of matching heat sources and heat sinks. Our preliminary efforts towards this goal show a good agreement with experimental data.

The study of the influence of operating parameters on the optimal design and achievable process performance shows that there are subtle tradeoffs and advanced design tools such as optimization are crucial. The superstructure contains both mixing and splitting of streams as well as inherent nonlinearities, such as the heat losses, and therefore the full model will most likely result in a nonconvex mixed-integer nonlinear program (MINLP). Because there are a number of operating conditions and modeling parameters which are not accurately known, tools like parametric or stochastic optimization will very likely provide new insights on the optimal design and its flexibility and robustness.

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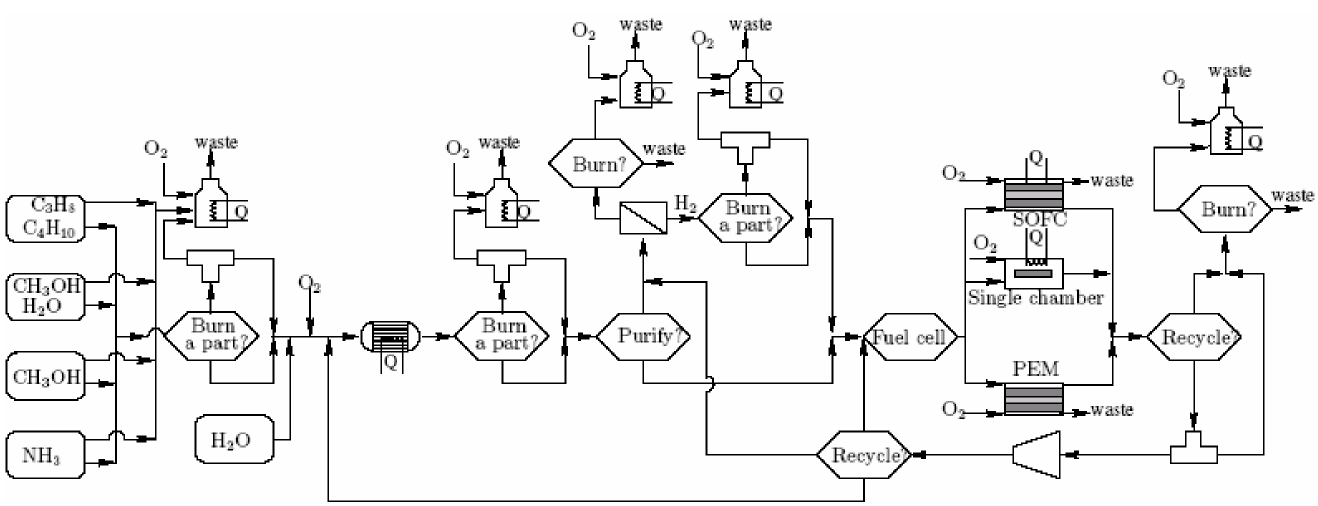

Figure 1: Process superstructure