

497a Optimal Start-up of Micro Power Generation Processes Employing Fuel Cells

Benoit Chachuat, Alexander Mitsos, and Paul I. Barton

The widespread use of portable electric and electronic devices increases the need for efficient autonomous man-portable power supplies (up to 50 W). 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. 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 and the upper limit on performance is now being reached. A promising alternative is to use common fuels/chemicals such as hydrocarbons or alcohols and there is a great military [1] and civilian interest, e.g., [2], in developing battery alternatives based on these fuels and portable fuel cell systems.

The work presented in this paper is part of a systematic design methodology for portable power generation based on fuel cell systems. The devices considered have characteristic dimensions ranging from the submicron level for membranes up to a few millimeters for the fuel cell length (inner dimension) while the overall system size including packaging is restricted to centimeters at the most. The necessity for such a methodology is warranted due to the plethora of possible processes and process combinations, as well as the wide variety of applications and consumers, ranging from cellular phones and laptops for home use to the power needs of the dismounted soldier. Moreover, there is a strong interaction between design and operation (steady-state and dynamic) which leads to various counter-intuitive effects [3] and therefore makes a systematic design methodology employing models, simulation and mathematical programming, as opposed to empirical design based on trial-and-error, necessary.

Since most power consuming devices are not operated constantly and have rapidly changing power demands, the dynamics and automated operation of portable power production are very important and must be considered thoroughly. The processes must operate fully autonomously and automatically without the intervention of operators. Operational considerations are indeed so important that they are likely to influence the optimal design, following the paradigm of interaction of design and operation. For example, it might be necessary to oversize certain units relative to optimal steady-state design, or exclude processes that exhibit poor transient behavior.

The focus of this presentation is optimal transient operation of microfabricated fuel cell systems for man-portable power generation. We are using intermediate fidelity models for the simultaneous optimization of design and operation (steady-state and transient) for a given process structure, which can be obtained from a system level analysis [4]. A particular strength of the models developed is that there is no need for the specification of a detailed geometry. The models used are rigorous based on validated kinetic models and therefore these type of models are particularly useful for technologies with demonstrated proof-of-principle. We have therefore studied processes based on ammonia decomposition and butane combustion, and we are currently considering butane partial oxidation. Our focus has been on high temperature solid oxide fuel cells which have the benefit of fuel flexibility. For the moment we are considering start-up with an auxiliary battery as opposed to ignition reactions.

In particular, the optimal start-up of the processes is of great interest. It is most likely that the devices will be coupled with a relatively small rechargeable battery for start-up and shut-down operations. Objectives for the optimal start-up procedure include minimization of the time required to reach steady-state and minimization of the overall system mass and volume. Constraints include structural stability considerations which map mainly into constraints on temperature, temperature gradients and its time derivatives as well as requirements regarding the emission of toxic gases.

Detailed models of the complete operating cycle exhibit hybrid discrete continuous behavior, because different operating modes, e.g., discharging and recharging of the battery, are described by different models. The models involve partial differential-algebraic equations and no algorithms exist that guarantee the global optimization of such problems; therefore we mostly employ local optimization techniques. The partial differential equations have multiple time scales and we have developed numerical techniques based on separation of scales to allow efficient integration of the state and sensitivity equations.

The optimal start-up consists of three phases. In the first phase the battery is used to meet the power demand as well as to heat up the fuel cell stack. In the second phase the battery is used to only meet the power demand while butane is burned to further heat up the stack. In the last phase the fuel cell stack is operated at a higher load than steady-state to meet the power demand as well as to recharge the battery; for this an increased flow of fuel is required resulting in a temperature higher than steady-state. The implication of the start-up for design is that the sizing of the reactor/fuel cells needs to take into account the start-up phase where power is generated to recharge the battery.

[1] R. Jacobs, H. Christopher, R. Hamlen, R. Rizzo, R. Paur, and S. Gilman. Portable power source needs of the future army - batteries and fuel cells. *IEEE AES Systems Magazine*, 11(6):19--25, 1996.

[2] Charles Mann. Near-term nanotech. *Technology Review*, page 22, July/August 2004.

[3] Benoît Chachuat, Alexander Mitsos, and Paul I. Barton. Optimal design and steady-state operation of micro power generation employing fuel cells. *Chemical Engineering Science*, 60:4535--4556, 2005.

[4] Alexander Mitsos, Michael M. Hencke, and Paul I. Barton. Product engineering for man-portable power generation based on fuel cells. In Press: *AIChE Journal*, Nov 2004.