570a A Design and Operation Methodology for Man-Portable Power Generation

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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, e.g., [2], interest in developing battery alternatives based on these fuels and portable fuel cell systems.

In the recent past microchemical systems have received special attention [3] and dramatic improvements have been made. Chemical units such as reactors, separators and fuel cells with feature sizes in the submilimeter range are being examined for a variety of applications. Microchemical systems have several advantages compared to macro-scale processes: the increased heat and mass transfer rates at the micro-scale allow higher yields [4]; the small hold-up along with the controlled conditions allow reaction pathways deemed too dangerous for conventional processes; the small quantities required and the possibility of parallelization have sparked interest in the micro-total-analysis-systems (lab-on-a-chip) [5]. Currently most of the microreactors are not standalone devices, but rather are used within a conventional laboratory.

The replacement of batteries for electronic devices requires truly man-portable systems and therefore the use of microfabrication technologies is plausible since a minimal device size is required. Most of the research in micropower and microreaction technology has focused on fabrication techniques or detailed modeling whereas there are still few contributions regarding design methodologies for such systems.

This paper presents an integrated design methodology for portable power generation based on fuel cell systems. The necessity for such product design 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. The strong interconnection of design and operation (steady-state and dynamic) and the complexity of the systems lead to various counter-intuitive effects and therefore make a systematic design methodology employing mathematical models, simulation and optimization as opposed to empirical design based on trial-and-error, necessary. 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.

With current computational possibilities and available algorithms it is impossible to solve for the optimal design and operation in one step since the devices considered involve complex geometries, multiple scales, time-dependence and parametric uncertainty. Therefore, our methodology is based on decomposition into three levels of modeling detail, namely system-level models for process synthesis, intermediate fidelity models for optimization of sizes and operation, and computational fluid dynamics detailed models for geometric design. While our work is mainly theoretical it allows and employs interactions within a multidisciplinary research group at MIT; experimentally determined parameters are used in our models and the optimal design and operation obtained are used in the fabrication efforts. Moreover, although our models are tailored to micro-fabricated fuel cell systems the aforementioned methodology can be applied to generic products that involve physico-chemical processes.

Process synthesis and layout considerations are performed with the use of algebraic models that are general enough to be independent of the catalysts used. Through the use of simulation and parametric mixed-integer optimization the most promising process structures along with idealized layouts are selected among thousands of alternatives [6,7]. We are considering a variety of fuels including hydrogen, ammonia, various hydrocarbons and alcohols, and fuel cells including solid oxide fuel cell (SOFC), polymer electrolyte membrane (PEM), single chamber solid oxide fuel cell, direct methanol fuel cell (DMFC) and proton conducting fuel cell based on ceramic technology (PCFC). The optimal process structure depends on technological advances and product specifications. The system level analysis provides limits of performance and can be used to determine at an early stage if a proposed device is worth pursuing; as an example the use of methane, which has been proposed in the literature, is shown to be marginally competitive with existing battery technologies, because of the storage requirements.

At the intermediate fidelity level we use distributed models, which allow optimization of unit sizes and operation (steady-state and transient) for a given process structure without the need to specify a detailed geometry. The resulting models involve partial differential-algebraic equations and the mathematical programming formulations employed include global and local dynamic optimization as well as stochastic programming [8,9]. The models used are rigorous based on validated kinetic models. This level of modeling detail is particularly useful for technologies with demonstrated proof-of-principle. So far we have studied processes based on ammonia decomposition and butane combustion, and we are currently turning our attention to butane partial oxidation. Our focus has been on high temperature solid oxide fuel cells which have the benefit of fuel flexibility.

Finally, the use of detailed two- and three dimensional computational fluid dynamics allows geometrical improvements as well as the derivation and validation of modeling assumptions that are employed in the system-level and intermediate fidelity models. The development of these models requires specification of the geometry and therefore benefits from the collaboration with fabrication efforts. Since the convergence of such models is time consuming and not robust, it is only possible to consider small variations in the geometry and this is done based on simulations as opposed to mathematical programming formulations. One of the major findings from CFD models was that for a class of devices the temperature profile in the active regions (reactor, etc.) is essentially uniform; this was also supported by scaling analysis and preliminary experimental results.

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