Design Course for
MICROPOWER GENERATION DEVICES

ALEXANDER MITSOS
Aachen Institute for Advanced Study in Computational Engineering Science, RWTH Aachen • Aachen, Germany

The chemical engineering field of study is undergoing changes, with more focus on emerging areas in molecular chemistry and biology, product design, and micro- and nanotechnology. On the other hand, design courses are still considered the capstone of an undergraduate chemical engineering program. This article describes a recently developed course for the Department of Chemical Engineering at the Massachusetts Institute of Technology (MIT) and the Aachen Institute for Advanced Study in Computational Engineering Science (AICES) at the RWTH Aachen. The course considers the design of microfabricated fuel cell systems for man-portable power generation.

The term man-portable is defined as: capable of being carried by one person, typically over long distance, without serious degradation of the performance of that person's normal duties. Efficient alternatives to batteries for man-portable power generation are necessitated by the ever-increasing use of portable electric and electronic devices. The desired power level is in the order of 0.5 to 50W. There are several reasons for replacing batteries. In addition to their high cost and large life-cycle environmental impact, batteries have relatively low gravimetric (Wh/kg) and volumetric (Wh/l) energy density. State-of-the-art rechargeable batteries reach only a few hundred Wh/l and Wh/kg. Battery performance has significantly improved over the last decades, but it is believed that the upper limit on performance is being approached, because the list of potential materials is being depleted. A promising alternative is to use common fuels/chemicals such as hydrocarbons or alcohols as an energy source.

There is significant research activity in the area of microchemical systems.[1] Chemical units such as reactors, separators and fuel cells with feature sizes in the submillimeter range have been considered for a variety of applications, due to their advantages compared to macroscale processes, such as the increased heat and mass transfer rates.[2] The replacement of batteries for electronic devices requires man-portable systems and therefore the use of microfabrication technologies is plausible since a minimal device size is desired.

There is great military[3] and civilian interest in developing battery alternatives based on common fuels/chemicals such as butane. As a consequence, a lot of research projects have been undertaken in academia and industry (see, for example, References 4–6 for reviews). While there are well-established microchemical courses with emphasis on microfabrication, the author is not aware of any course with emphasis on process synthesis, process design, or optimization. Such a course is proposed herein; in addition to covering technological aspects of exciting topics (microchemical systems, fuel cells) it combines process and product design. This is important in view of recent trends for product-oriented design.[7–12] The course developed is based on several research publications of the Process Systems Engineering Laboratory at MIT.[13–21] In the

Alexander Mitsos *is currently a junior research group leader at RWTH Aachen. He received his engineering diploma from the University of Karlsruhe and his Ph.D. from MIT, both in chemical engineering. For both degrees he was awarded distinctions, prizes, and fellowships. He has more than two years of industrial experience, and has authored or co-authored more than 15 articles in refereed journals. His research includes microscale and macroscale energy systems and the development of global optimization algorithms.*

remainder of the article, first the contents of the lectures are described in Section 1, and then the project tasks are summarized in Section 2. The article concludes with the skills gained by students, scope of improvement for the class, and summary of the experiences from teaching the class.

1. LECTURE CONTENTS

The course duration is six weeks, with three hours of lectures per week. No textbook is available for the course, but the material covered in Reference 6 is the primary reference. Other useful references are books on microchemical systems, design, and thermodynamics.[22-26] Approximately one week of lectures is reserved for software tutorials and discussions of issues raised by the students during the project execution. The remaining five weeks are devoted to five topics, namely the introduction and motivation, aspects of fuel cells, process synthesis, selection of alternatives, and process optimization. These topics are summarized in the following.

1.1 Introduction, Motivation, and Project Description

The first week of lectures is devoted to a description of the project as well as an introduction. These lectures are intended to give the students the big picture of the project and help them understand the goals of their tasks. First, the motivation for micropower generation is given. This is done by comparing the trends in power consumption by portable electric devices and electronics to the performance characteristics of batteries. Pricing and performance of batteries are discussed, along with their environmental impact. A common critique to fuel cell-based systems for micropower generation is that they are deemed too dangerous. To put these claims into perspective the safety issues of batteries (fire, explosions, etc.) are discussed and demonstrated by pictures and movies.

The next step in the introduction is the definition of the key metrics for man-portable power generation devices, namely the gravimetric and volumetric energy densities

$$e^{sys}_{grav} = \frac{\tau_{mission}\,PW}{M^{sys}}, \qquad e^{sys}_{vol} = \frac{\tau_{mission}\,PW}{V^{sys}}, \tag{1}$$

where the mission duration $\tau_{mission}$ (h) is the time between refueling or recharging, PW (W) is the power output (assumed constant for simplicity), M^{sys} (kg) is the mass of the system, and V^{sys} (l) is the volume of the system. These metrics are typically the objectives to be maximized by the process synthesis design and operation. In cases where the mission duration is very long and the device miniaturized, the size of the system is dominated by the fuel cartridge, in which case the simpler metrics of fuel energy density can be used:

$$e^{fuel}_{grav} = \frac{PW}{3600\sum_i MW_i N_{i,in}}, \qquad e^{fuel}_{vol} = \frac{PW}{3600\sum_i MV_i N_{i,in}}, \tag{2}$$

where $N_{i,in}$ (mol/s) is the inlet molar flowrate of species i, MW_i (kg/mol) is the molecular weight of species i, MV_i (l/mol) is the molar volume of species i at storage conditions, 3600 is the conversion factor from hours to seconds, and the summation is taken over all stored fuels and oxidants.

In man-portable power generation the most important advantage of microfabrication is device miniaturization. Microfabrication techniques are outside the scope of the course. On the other hand, various examples from microchemical systems are analyzed with emphasis on entire systems as opposed to components. The importance of physical phenomena at the microscale is analyzed and compared to the macroscale; for instance, it is shown that viscous forces dominate over inertial forces and that heat transfer (and loss) has much more importance than in the macroscale. Various alternatives for man-portable power are summarized, such as microturbines[27] and devices based on man-power.[28]

A common critique of micropower generation devices, and particularly of high-temperature systems, is that they pose safety threats and generate a lot of heat. These concerns are analyzed via back-of-the-envelope calculations. It is argued that these concerns are partially true and partially misconceptions resulting from macroscale experience. The high energy density of the fuels is of concern, as is the use of toxic fuels. On the other hand, the use of high-temperature devices is not a safety hazard, because of the low heat capacity and the insulation.

1.2 Fuel Cell Working Principles and Types

Both the batteries and the fuel cell systems studied, *i.e.*, the product to be replaced and the proposal for replacement, rely on electrochemical reactions. Electrochemistry is covered in some undergraduate curricula, but not in sufficient detail for performing and understanding the project tasks. Therefore, the principles of fuel cells are briefly summarized, along with a repetition of the relevant concepts from reactor engineering and thermodynamics. Then, the thermodynamic limits of fuel cell performance are analyzed and compared to heat engines.

Several fuel cells technologies have been proposed over the last decades. Some of the fuel cell types have a potential for scale down, such as solid-oxide fuel cells (SOFCs), polymer-electrolyte membrane fuel cells (PEMFCs) operating with hydrogen, direct methanol fuel cell (DMFC), proton ceramic fuel cells (PCFC), and membrane-less fuel cells, *e.g.*, References 29–31. Miniaturization has been performed for some of the fuel cell types, often with the use of microfabrication technologies. These fuel cell types are analyzed with an emphasis on advantages, disadvantages, and operating characteristics.

1.3 Conceptual Process Design at the Macroscale

Process synthesis at the macroscale is typically included in undergraduate curriculum. In the proposed course a brief summary of the techniques and methodologies is given, with emphasis on superstructure-based approaches.[25] This is deemed helpful for the students to be able to compare the challenges with the selection of alternatives at the microscale. For instance, the discussion of heat exchanger network synthesis demonstrates that at the microscale the challenges are very different: no utility streams are available, and the operating conditions of various components are not independent from each other due to the pronounced heat transfer. In addition, having this short summary allows students from different disciplines to attend the course. The lectures also briefly discuss some of the mathematical and algorithmic background used in conceptual process design. The emphasis is on the material that is relevant to the project tasks.

1.4 Selection of Alternatives

A major challenge in the system design of micropower generation processes is the selection of alternatives, in particular which fuel to use for power and/or heat generation, what fuel cell type to select, whether a fuel reforming path should be followed and how heat integration should be performed. This selection of alternatives at the microscale is analogous in principle to macroscale process synthesis. Moreover, some of the mathematical techniques used in macroscale process synthesis can also be used for the selection of alternatives. There are several major differences, however, including different objectives and constraints and the fact that the unit operation paradigm must be replaced by that of highly integrated components in a system.[32] An additional challenge is the early stage of technology development.

The lectures describe the large number of alternative processes arising from the large choice of fuels, fuel reforming reactions, and fuel cells. The advantages and disadvantages are discussed and a system-level approach for modeling is detailed.[13, 14] This modeling approach is then used in one of the projects offered, see Section 2.1. The advantage of this methodology is that the most promising alternative(s) can be selected without detailed knowledge about the technological details, such as the catalysts used or the reactor configuration. The disadvantage is that some parameters, which in principle can be calculated, are viewed as input parameters—*e.g.*, the fuel conversion in the reforming reactor for a given operating temperature and residence time.

1.5 Optimization of a Given Process Alternative

Once a promising alternative has been chosen, the design and operation can be optimized via models of intermediate fidelity.[15-19] The spatial discretization results in problems with (partial) differential-algebraic equations. The models employ spatial discretization when necessary and are based on first-principle models. As a consequence they are predictive and can be used to find the optimal sizing of units (reactor, fuel cell, etc.) as well as operating variables (voltage, temperature, flowrates, etc.). A drawback is that the development of such a model takes significant effort and requires knowledge of kinetic rates.

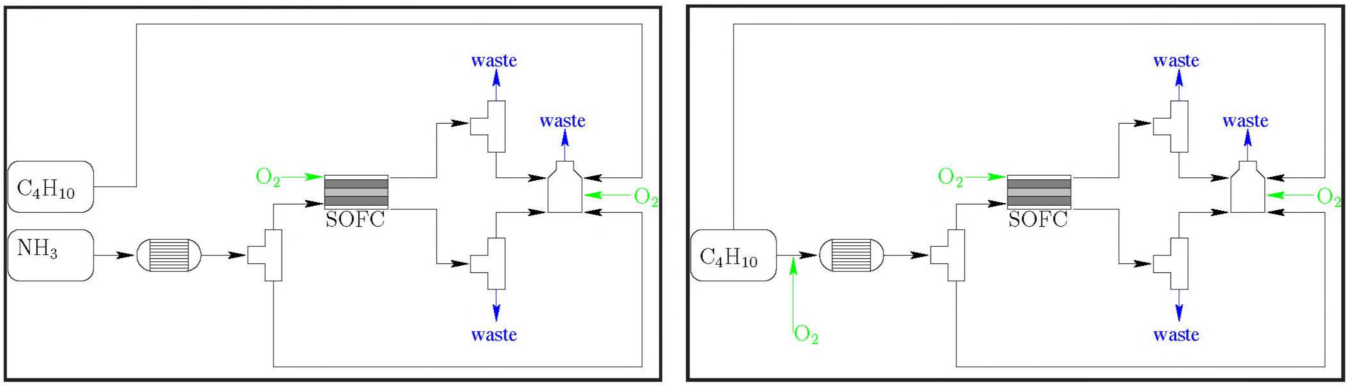
For the optimization of design and operation, algorithms from mathematical programming with differential-algebraic equations (DAEs) embedded can be used. These techniques are briefly described in the lectures along with techniques for the simulation of DAE systems. The state-of-the-art in dynamic optimization, however, is such that the use requires significant mathematical background and computational experience, and is deemed limitedly suitable for an undergraduate class in chemical engineering. Instead, in the project (Section 2.2) the optimization is based on a simulation approach, in which the students must specify the degrees of freedom. To simplify the problem, some variables (such as the operating temperature and voltage) are prespecified. On the other hand, to give some experience in the use of advanced methods, the simpler problem of parameter estimation is given as a subtask to be solved with an optimization algorithm.

2. DESCRIPTION OF PROJECTS

Two alternative projects are offered. The recommendation is to offer these in alternate years. Offering both projects in parallel (to different groups of students) is also possible, however it complicates logistic considerations significantly, since the material necessary for the project must be covered in class prior to the project assignment. A third alternative would be to assign both projects, and extend the course duration.

2.1 Selection of Alternatives

Two main processes are considered, see Figures 1. Both are



Figures 1. *Process flow sheets for project on selection of alternatives.*

based on a solid-oxide fuel cell (SOFC); one of them uses NH_3 as the fuel for power generation while the other uses C_4H_{10}. All units are modeled using stoichiometric reactors, *i.e.*, a fixed conversion is assumed for each reaction. As a consequence, relative rough estimates for the process performance are obtained; however, these estimates are sufficient for a comparison of alternatives. All units are microfabricated on a single silicon chip; as a consequence they share the operating temperature of T = 1000K. The entire process operates at ambient pressure. The gas phase is assumed to be ideal. A power production of 10W is requested. The enthalpy of the inlet streams is calculated at ambient conditions and the gaseous phase. For the outlet streams a temperature of T_{out} = 600K is assumed, based on heat recovery.

The models for the processes are given to the students as a Jacobian[33] input file. The students must perform additional calculations, such as the calculation of energy density based on the calculated flow rates. For these calculations the students have the choice of using Jacobian or a software tool of their choice.

2.1.1 Project Tasks

The first task is to optimize the processes based on NH_3 and on C_4H_{10}. The operational variables are the flow rates of fuel and the split fractions in the 3 splitters. The flow rates of air are a direct consequence of the fuel flow rates and a specified stoichiometric ratio. The objectives are to maximize the volumetric and gravimetric energy density; the device mass and volume can be ignored, but the fuel cartridges must be accounted for.

The second task is to compare the optimized processes with a conceptual process based on methane, stored at ambient temperature. An overall efficiency (power produced divided by chemical energy consumed) of 50% is assumed. The main challenge is to calculate the required cartridge thickness and volume as a function of pressure for various container types, *e.g.*, plastic or steel.

The third task is to compare the optimized processes with a process based on an H_2 generator, such as a hydride. The goal of this task is to identify the storage properties (hydrogen volume % and density) required to match the best process in terms of both gravimetric and volumetric energy density. To do so, an overall efficiency of 70% is assumed.

2.2 Optimization of NH_3-Based Process

The project task is to optimize a micropower generation device for the production of PW = 10W. A fixed process is considered based on NH_3 cracking to H_2 and electrochemical oxidation of the produced H_2 in a solid-oxide fuel cell (SOFC). The device comprises two parallel lines, namely the NH_3 line for power generation and the C_4H_{10} line for heat generation, see Figure 2. These two lines are not independent, because they are microfabricated in a single silicon chip; as a consequence they share the operating temperature of 1000K. The entire process operates at ambient pressure. The gas phase is assumed to be ideal. The model considers one-dimensional spatial discretization and a kinetic model for the catalytic reactions. All assumptions for the model have been shown to be valid (see Reference 15).

2.2.1 Project Tasks

The first project task is to determine appropriate values for the constants in the kinetic rate of NH_3 cracking, by fitting to a set of experimental values. The students are given a postulated kinetic mechanism along with experimental data of conversion as a function of residence time for four different temperatures. The kinetic mechanism has two adjustable parameters and the data contain random error. The students must extend an example provided to them. This task is relatively simple, thanks to the estimation capabilities of Jacobian.

The main task of the project is to maximize the energy density of the device; this is done by optimizing the volumes of the device components and the flowrates of fuel and air. There are four design variables, namely the volumes of the reactor, SOFC, hydrogen burner, and butane burner. In addition, there are also four operational variables, namely the feed flowrates of fuel (NH_3 and C_4H_{10}) and air (to the SOFC and to the butane burner). The temperature and voltage have been fixed. The optimization is a challenging task, in which the students can only succeed if they employ a systematic procedure for varying the variables. The achievable energy densities are significantly higher than in state-of-the-art batteries; however this requires successful optimization of the process design and operation.

The final task is to analyze potential improvements to the process. This analysis includes the comparison of the chosen process configuration with alternatives, such as using stored oxygen and having a fresh-air stream to the burner instead of using the cathode effluents. The students are also asked to comment on the effect of increasing or decreasing the temperature and the voltage. The process relies heavily on catalysts, and not surprisingly the performance of catalysts significantly

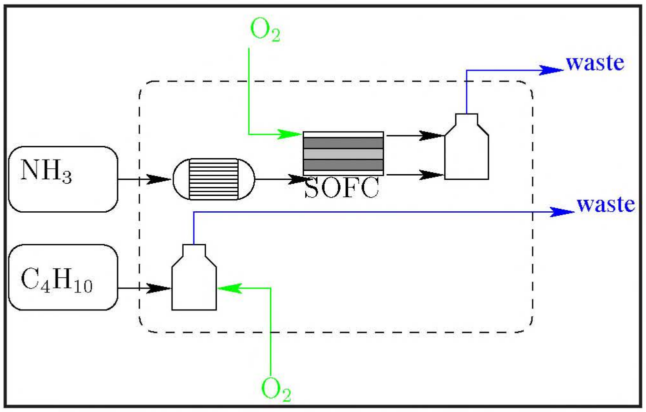


Figure 2. *Process flow sheet for project on process optimization.*

affects the overall process performance; the students are asked to identify which component is the most important to optimize (reactor, burner, or fuel cell). Finally, the students are asked to explain how a doubling of the desired power demand level will affect the process design and operation.

3. CONCLUSIONS

A new course on the design of microfabricated fuel cell systems is offered for chemical engineering students.

The course is project-based and spans six weeks. The theoretical material needed for a successful project execution is covered in three lectures per week, each one-hour long. The students learn several skills through the lectures and project. Likely the most important skill is learning how to work in a team, as in any course based on group projects. The most important technical skills are process and product design, and in particular their interaction. The students have a chance of integrating the knowledge acquired in their preparatory classes, especially thermodynamics and reactor engineering. Finally, the students are familiarized with the exciting technologies of fuel cells and microchemical systems.

The course was developed for chemical engineers. The class was first offered in Spring 2008 at RWTH Aachen. The format of the class was a seminar for graduate students with backgrounds in mechanical and chemical engineering. Approximately five students attended the lectures, which is a typical size for seminars. No project was offered. The full class, including the project, is currently offered at MIT. It is one of the elective modules in Integrated Chemical Engineering. More than 20 students, corresponding to approximately one third of the class, chose this module. This is a success, given that the course is offered for the first time. Class evaluations are not available yet, but the preliminary informal feedback from the students is also very positive. A potential extension would be to aim at interdisciplinary class. In particular it would be interesting to consider teaching joint classes in chemical, mechanical, material, and electrical engineering.

In the lectures and project, material and structural considerations are taken into account as simple constraints, *e.g.*, a maximal operating temperature. It would be interesting to incorporate the interaction of these considerations with process design and optimization more thoroughly. This is currently not possible, since the effect has not been examined sufficiently in the literature. Moreover, incorporating such structural and material considerations in a chemical engineering class would be very challenging.

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