

Optimal Start-up of Micro Power Generation Processes

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Abstract

Fuel cell based systems are a promising alternative to batteries in man-portable power generation applications. These micro power generation processes must operate fully autonomously and automatically without the intervention of operators. Operational considerations are indeed so important that they influence the optimal design, following the paradigm of interaction of design and operation. This paper presents a methodology for the simultaneous optimization of design and operation of such systems. We illustrate the methodology with two case studies, focusing on the start-up procedure. A small rechargeable battery is necessary to satisfy the power demand during the start-up while the device temperature is too low for power generation. The optimization problem is formulated as minimization of the mass of fuel and battery required to heat the device up to operating temperature.

Keywords: man-portable power; micro power generation; micro fuel-cell system; optimal start-up operation; dynamic optimization

1. Introduction

The widespread use of portable electric and electronic devices increases the need for efficient man-portable power supplies (up to 50 W). Currently, batteries are the predominant technology in most applications, even though they have a large environmental impact, high cost and relatively low gravimetric and volumetric energy densities; furthermore, the upper limit on performance is now being reached. Out of the alternatives that are possible, we are focusing on micro scale power generation devices based on the electrochemical conversion of common fuels and chemicals, such as hydrocarbons or alcohols, in fuel cells. These process-product hybrids have the potential to yield much higher energy densities than state-of-the-art batteries, because the above mentioned fuels have very high energy contents and fuel cells can in principle achieve very high efficiencies.

Since most power consuming devices are operated periodically and have rapidly changing power demands, the dynamics and automated operation of portable power production are very important and must be considered thoroughly. In this paper, the focus is on the optimal start-up of micro power generation processes. It is most likely that the devices will be coupled with a relatively small, rechargeable battery; its role is to ensure that the power demand is met when the fuel cell is unavailable or can only

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satisfy part of the demand, to provide the energy needed to heat the stack up to a temperature at which chemical and electrochemical reactions are fast enough, or to provide an electric spark for the initiation of a combustion reaction.

2. Methodology

Our methodology relies on the assumption that intermediate fidelity models can approximate the performance of the devices and can be used for optimization purposes. Our models do not require the specification of a detailed geometry and rely mainly on first-principles, containing only a minimal number of modeling parameters. This is possible because the relative importance of physical phenomena at the micro scale makes one-dimensional spatial discretization sufficient.

We assume that the molar flux in the gas channels of the fuel processing reactor, fuel cell and burners is convective in the flow direction (PFR), and axial diffusion can be neglected; on the other hand we assume that diffusion in the radial direction is fast enough to ensure a uniform profile in the cross-section. These assumptions have the consequence that micro-fabricated units such as reactors or fuel cells can be approximated by an idealized model using 1-D species balances, without the inclusion of the diffusion term. We neglect the pressure drop along the gas channel and assume an ideal gas. Back-of-the-envelope calculations based on the expected device dimensions using Hagen-Poiseuille's equation provide an estimated pressure drop in the order of a few kPa, i.e., a relative pressure drop of a few percent only. We note that this value is in good agreement with the measurements for a micro-fabricated reactor made by Arana (2003). As a consequence, no solution of momentum equations is necessary. We further assume that heat transfer is fast enough, so that the temperature throughout the device, or regions of the device, is near uniform. This is typically the case at the micro-scale for silicon based reactors. Finite element simulations were also performed, which confirm this assumption. It is important to note that considering a uniform temperature allows one to not specify a particular geometry for the unit operations and their arrangement in the stack. Otherwise, not only the generality of our study would be inherently affected, but problems would also be encountered as several micro devices and components of the proposed processes are not fully developed thus far. Due to material constraints and technological limitations the start-up time will be in the order of at least one minute, much longer than the residence time of gases in the process, which is in the order of ms. We therefore assume pseudo-steady-state concentration profiles along the various units at each time instant. This assumption allows us to solve the concentration profile at each time step using an integration along the spatial axis, similar to the steady-state case (Chachuat *et al.*, 2004) without requiring method of lines semi-discretization of the state variables; in some cases this assumption even allows the calculation of analytical solutions for the concentration profile. It should be noted that if one wanted to explicitly calculate the material stresses developed, a fully transient model would be necessary.

The objective of the start-up problem is to bring the fuel cell to its nominal temperature while minimizing the total mass (battery and fuel) required for this heat-up and meeting the nominal power demand at all times. In the case studies we assume that the battery

can also be used for heat-up of the device. Additional constraints can also be specified, such as a maximum rate of change for the temperature based on structural stability considerations, or requirements concerning the emission of toxic gases. Since different operating modes are described by different sets of equations (e.g., discharging and recharging of the battery), the start-up problem is formulated as a hybrid discrete/continuous dynamic optimization problem (Lee and Barton, 2002). This optimization problem is solved by using recent developments in numerical methods for dynamic optimization with hybrid systems embedded.

3. Case Studies

3.1. Case Study 1: Butane Based Process

A very promising process for micro power generation is the partial oxidation of butane, with subsequent electro-chemical conversion of the generated syngas in a Solid Oxide Fuel Cell (SOFC) (Mitsos *et al.*, 2004a); one of the main advantages of this process is that butane has a very high energy content, and partial oxidation is an exothermic reaction. Therefore, oxidation of the fuel cell effluents is sufficient to overcome the heat losses at steady-state operation. A conceptual flowsheet for the process is shown in Figure 1; the reactor, fuel cell and catalytic burner are assumed to be thermally coupled and operate at a common uniform temperature. The drawbacks of this process are that butane partial oxidation has not yet been demonstrated at the micro-scale and limited kinetic data are available; therefore the model presented should be considered preliminary and the results qualitative rather than quantitative.

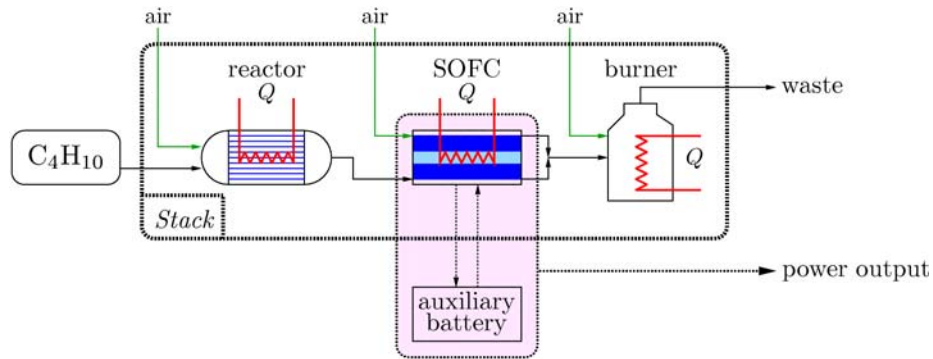


Figure 1. Conceptual flowsheet for butane based process.

We now present results obtained from optimization of the butane based process at a nominal power output of 1 W and a nominal operating temperature of 1000 K. Figure 2 illustrates the optimal profile, obtained by applying a piecewise constant approximation with 50 control segments of equal duration to solve the problem. The optimal start-up procedure duration was determined to be around 150 s. The number of time intervals has an insignificant influence on the start-up performance in terms of the objective function.

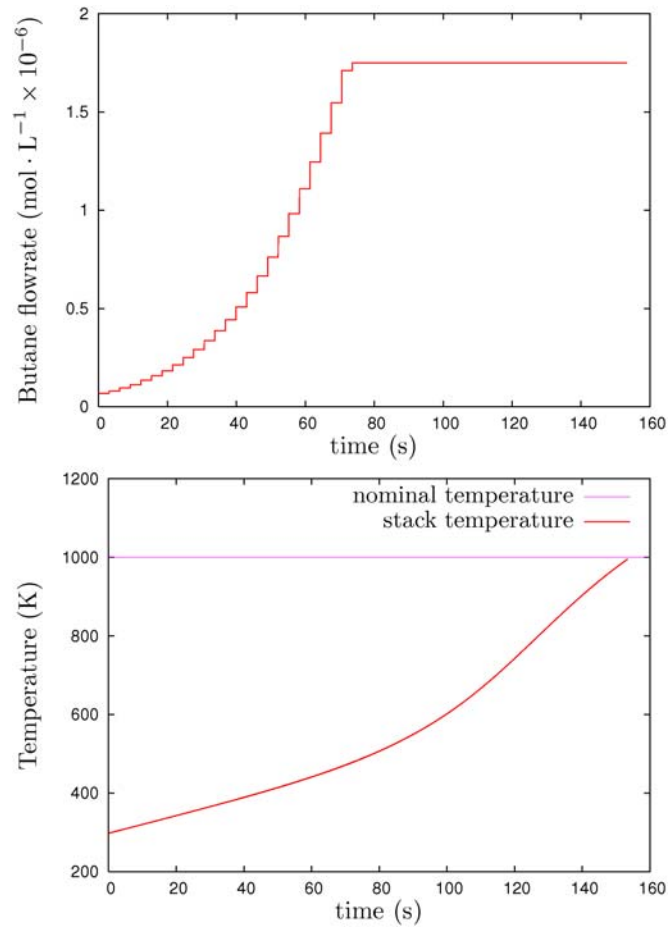


Figure 2. Time profiles for optimal start-up of butane process.

3.2. Case Study 2: Ammonia Based Process

Ammonia is often considered as a potential energy source in fuel cell systems, e.g., Metkemeijer and Achard (1994), because ammonia decomposition produces hydrogen. A drawback of this process is that ammonia is corrosive and toxic and therefore tight constraints regarding the emission of residual ammonia need to be imposed. Also, ammonia decomposition is an endothermic reaction and therefore a heat source is required. While oxidation of part of the hydrogen produced could be used to provide the necessary heat, a more promising approach Mitsos *et al.* (2004b) is the use of a secondary fuel with a high energy density, such as butane. In Chachuat *et al.* (2004), we have considered optimal steady-state operation of the process shown in Figure 3 and we now extend this work to transient operation.

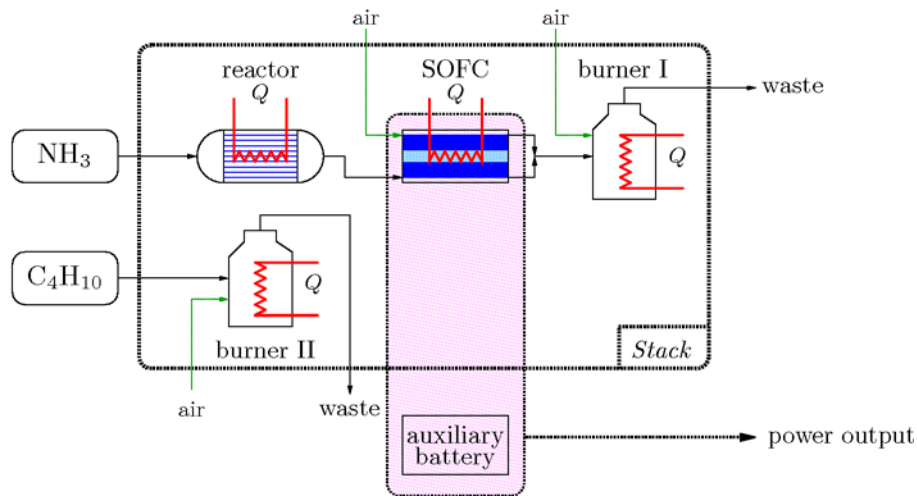


Figure 3. Conceptual flowsheet for ammonia based process.

The scope of this paper does not permit a detailed discussion of the start-up procedure for the ammonia based process. Instead we present how, for a fixed design, the fuel energy density (in Whr/Kg) changes as a function of the power output. This consideration is very important for the transient operation, since at start-up it is plausible to gradually increase the flow through the fuel cell. Furthermore, the power demand of power consuming devices is time varying and there is a trade-off between running a process away from its optimal operating point and consuming more energy from the auxiliary battery. In Figure 4 the design optimized for a nominal power demand of 10 W (Chachuat *et al.*, 2004) is used and the energy density based on optimal steady-state operation is shown in comparison to the design optimized for the given power output. It should be noted that we do not consider a variation of the operating temperature, assuming that the design was done for the maximal allowable temperature, based on material constraints. The energy density is maximal at a power demand slightly higher than the one for which the system was designed (≈ 10.1 W). For power demands lower than the design power output, the heat generation is small, and relatively more butane needs to be burned to compensate for the heat losses. For an increasing power output, the ammonia flowrate is increased and the fractional conversion in the reactor and fuel cell is decreased; the constraints on residual concentrations of ammonia and nitric oxide in the outlets are only met with a largely increased flow of oxygen, which results in higher requirements for heat and a higher butane flow rate. The flow rate for oxygen quickly becomes so large that the pressure drop through the system would become significant, making the process practically infeasible and also violating one of our main modeling assumptions. This case study shows that it is necessary to consider variations in the power demand during the design of the system, and a promising method is stochastic optimization.

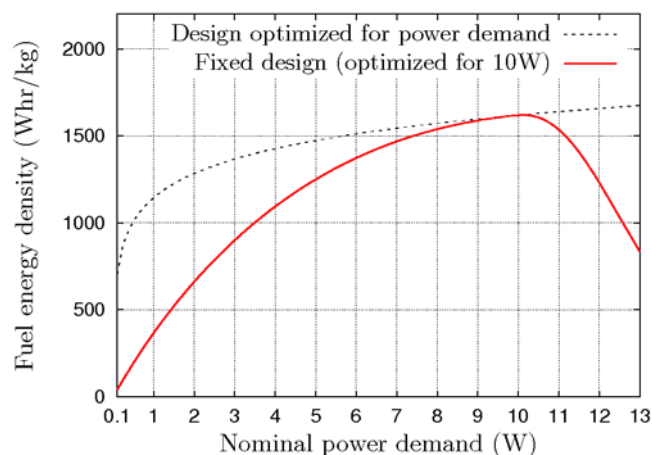


Figure 4. Process performance outside its optimal operating region.

4. Conclusions

A methodology for the simultaneous design and operation of fuel-cell based micro power generation devices was presented and demonstrated by considering the start-up procedure for two fuel-cell systems based on fuel processing in conjunction with a Solid Oxide Fuel Cell. The models used are of intermediate fidelity, allowing the optimization of design and operation without the specification of an exact geometry. The formulated methodology allows the solution of the formulated problems using dynamic optimization tools. The case studies show a strong interaction between design and operation. We are currently extending our methodology and case studies to the whole operating cycle as well as varying power demands. We anticipate that using stochastic optimization formulations will allow a significant improvement in process performance.

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