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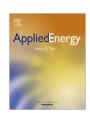
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Effect of operating parameters on the transient performance of a polymer electrolyte membrane fuel cell stack with a dead-end anode

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HIGHLIGHTS

- Experimental and computational study of PEM fuel cell stack with a dead-end anode.
- Investigation of the fuel cell performance, gas and water management.
- Gas and water management is better under low operating current conditions.
- Lower cathode stoichiometry is preferred to minimize nitrogen crossover.
- Anode purging is recommended to clear out the impurities for longer operations.

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ABSTRACT

The operation of polymer electrolyte membrane fuel cell (PEMFC) stack with a dead-end anode requires careful consideration on the gas and water management. Water accumulation at the anode and the nitrogen crossover from cathode to anode lead to performance deterioration over time. The accumulated water and nitrogen need to be removed properly by purging method to ensure good and stable stack performance. Thus, the careful selection of the operating parameters – inlet humidification, stoichiometry, and operating current – is the key factor for ensuring efficient water and gas management. This study aims at the experimental and numerical evaluation of the effect of the key operating parameters on the transient performance of a dead-end anode fuel cell stack. The experiments were carried out on a stack with 24 cells and a catalyst active area of 300 cm². By employing a validated transient two-phase mathematical model of a PEMFC with a dead-end anode, numerical simulations were performed which yield a better and deeper understanding of local distribution of water and species, i.e., hydrogen, oxygen, water vapor and nitrogen.

The results suggest that the performance deterioration over time is closely related to the choice of the operating conditions. The study reveals that the anode and cathode inlet conditions become a limiting factor for the stack performance. Liquid accumulation at the anode is found to be strongly related to the inlet humidification as well as water transport across the membrane, whereas the cathode stoichiometry affects the nitrogen crossover.

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1. Introduction

In a polymer electrolyte membrane (PEM) fuel cell with a deadend anode, effective and efficient gas and water management is vital in order to ensure optimal operation. In contrast to the open-end anode design, a higher utilization of hydrogen fuel is expected since there is no hydrogen excess to be wasted from the anode outlet as the anode outlet is sealed-off. However, water vapors may accumulate at the anode side and condense into liquid

which, in turn, blocks the hydrogen diffusion pathway and reduces the catalyst active area causing performance deterioration [1–4]. Furthermore, nitrogen can also crossover from the cathode to the anode side which causes impurities at the anode side and reduces the available hydrogen concentration for the electrochemical reaction since hydrogen is much lighter as compared to nitrogen [4–7]. These, in combination, lead to performance deterioration over time as has been frequently reported in the literature [1,3,4,8–10].

To recover the cell performance and to clear out the anode from the accumulated liquid and impurities, purging is the most common procedure in the dead-end anode operation. This is done by opening the anode outlet valve frequently to flush-out water and

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Nomenclature $\begin{array}{c} A_{\rm cl} \\ c_{\rm i}^{(\rm g)} \\ c_{\rm p}^{(\rm g)} \end{array}$ catalyst area, m² $p_{\rm H_2O}^{\rm sat}$ saturation pressure of water, Pa molar concentration of species i, mol m⁻³ liquid saturation specific heat capacity of gas mixture, J kg^{-1} K^{-1} S source term condensation/evaporation rate constant, s^{-1} T temperature, K $c_{\rm r}$ $\dot{D^{(c)}}$ capillary diffusion, m² s⁻¹ velocities, m s⁻¹ **u**, *u*, *v* diffusivity and effective diffusivity of species i, $\chi_{i}^{(g)}$ molar fraction of species i $m^2 s^{-1}$ *x*, *y*, *z* coordinates, m \mathbf{e}_{x} , \mathbf{e}_{v} , \mathbf{e}_{z} coordinate vectors $\omega_{\rm i}^{({\rm g})}$ mass fraction of species i cell and stack voltage, V $E_{\rm cell}$, $E_{\rm stack}$ heat of vaporization, J kg⁻¹ H_{vap} Greek i, i, $j_{\mathrm{a,c}}^{\mathrm{ref}}$ current density, A m⁻² porosity anode and cathode volumetric reference exchange over potential, V η current density, A m⁻³ $\dot{\theta}$ wetting angle volumetric current density, A ${\rm m}^{-3}$ permeability, m² к k thermal conductivity, W m⁻¹ K⁻¹ λ membrane water content I. length of channel, m dynamic viscosity, kg m^{-1} s⁻¹ μ interphase mass transfer due to condensation/evapo- $\dot{m}_{\rm H_2O}$ density, kg m⁻³ ration of water, kg m^{-3} s⁻¹ ρ $M^{(g)}$ conductivity S m⁻¹ σ mean molecular mass of the gas phase, kg mol⁻¹ potential, V electroosmotic drag coefficient $p^{(c)}, p^{(g)}$ capillary and gas pressure, Pa

impurities. However, this procedure may reduce the hydrogen utilization as some hydrogen may be lost during the purge and, to some extent, may lead to a potential fire hazard when it is mixed with oxygen from the ambient air. In addition, it also contributes to the complexity of the system design as it requires valves and control scheme and thus adds to the parasitic load of the fuel cell. Therefore, a careful balance between the purging frequency and the purging duration is essential to ensure the optimal fuel cell stack performance.

Several experimental [1-3,5,8-14] as well as numerical [4,15-17] studies have been performed to investigate the performance of the dead-end anode PEM fuel cell design. Manokaran et al. [12] experimentally studied the deterioration of the fuel cell performance and the nitrogen build up over time at the anode side using a segmented PEM fuel cell with the serpentine flow channel. They concluded that nitrogen accumulation is the major contributor for the performance drop. Choi et al. [13] introduced anode inlet pulsation to delay the purging time and reduce the accumulated liquid at the anode side. Wan et al. [14] proposed a method by condensing the vapor at the anode outlet to improve water management. In a previous work, Sasmito and Mujumdar [4] numerically investigated the local transport phenomena occurring during the dead-end anode operation and studied the effect of purging duration and frequency on the fuel cell performance together with the gas and water management. Recently, we also investigated experimentally the interaction between the purging frequency and duration as well as the cathode stoichiometry by employing the design of experiment (DoE) approach of fractional factorial study to search for the optimum combination of purging parameters [11]. Chen et al. [18] optimized the purge interval and cycle duration in a dead-end anode PEM fuel cell utilizing the along-channel, singlephase and transient dead-end anode PEM fuel cell model. Despite a wide range of studies conducted in the area of dead-end anode PEM fuel cell, none of them, however, has focused on the effect of operating parameters with respect to the transient performance and the local distribution of the accumulation of impurities at the anode side, which is the theme of this work.

To extend our work on the dead-end anode fuel cell, the purpose of this paper, therefore, is threefold: (i) to experimentally investigate the transient characteristics of a PEM fuel cell stack

operating in a dead-end anode mode; (ii) to numerically investigate the global and local distribution of gaseous species and water management with respect to the cell performance for the PEM fuel cell operating in a dead-end mode utilizing a validated transient two-phase model; and (iii) to evaluate the key operating parameters – operating current, inlet humidification and cathode inlet stoichiometry – during the transient operation of the PEM fuel cell with a dead-end anode.

The layout of the paper is summarized as follows. First, the experimental set up and measurements are introduced in Section 2. The mathematical model is outlined in Section 3, followed by the description of the numerical implementation in the commercial computational fluid dynamics software Ansys Fluent 13 utilizing the one-domain approach. The experimental polarization curves and cell voltage distribution throughout the stack are presented, after which the transient analysis on the experimental fuel cell performance is presented. The transient gas and water management are evaluated with help of the numerical analysis. Finally, conclusions are drawn with the emphasis on how the present results can aid in the selection of the operating parameters for good performance of a PEM fuel cell stack operating in a dead-end anode mode.

2. Experimental study

The PEM fuel cell test station used is a 24 cell, $300 \, \mathrm{cm}^2$ stack made by the Schatz Energy Research Centre (SERC); see Fig. 1 for details of the experimental setup. These fuel cells have a dead ended design and are operated under low pressure with a maximum power capacity of 1.5 kW. The stack is connected to a synchronized input/output data acquisition system that is controlled and monitored using a customized LabVIEWTM based software. The software allows users to setup the operating parameters. Also, it allows the user to setup the safety operation parameters to protect the stack form any operation fault that might occur in any of the stack cells. Air and hydrogen are supplied to the PEM stack using air cylinder (21.2% O₂, H₂O < 3.5 PPM, HC < 0.5 PPM, and the balance is N₂) and hydrogen cylinder (with 99.999% purity). Both gases are regulated to meet the stack demand at the standard conditions.

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