Water-Balance-Based Optimal Control for High-Current Operation of PEM Fuel Cells (Postprint)

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Abstract

Water management in proton exchange membrane fuel cells ((PEMFC) is one of the primary factors affecting their performance. This paper proposes a temperature control method based on IVIEA water balance for PEM fuel cells operating at high current densities. Under specific operating pressures and stoichiometric ratios, the water balance temperature of the PEM cell based on zero net electro-osmotic drag was obtained, and corrected through three-dimensional simulation to derive the operating temperature for optimal cell performance; the actual operating temperature control of the cell can be based on the zero net electro-osmotic drag water balance temperature curve, with a correction term added, to enable the cell to operate within a high-performance region. This cell operating temperature control algorithm is simple and provides a valuable reference for cell design and operation optimization.

Full Text

Preamble

The Optimal Control of PEM Fuel Cell Operating at Large Current Density Based on Water Balance

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Abstract

Water management in Proton Exchange Membrane Fuel Cells (PEMFC) is one of the key factors affecting performance. This paper proposes a temperature control method based on Membrane Electrode Assembly (MEA) water balance for PEMFC operated at large current density. For determined operating pressure and stoichiometry, the water balance temperature of PEMFC was acquired based on zero net electro-osmotic drag and subsequently modified through three-dimensional simulation, yielding an operating temperature based on optimal fuel cell performance. Actual temperature control of PEMFC can be carried out according to the water-balance temperature without net drag, modified by a correction amount, which helps the fuel cell operate in a high-performance region. This temperature control algorithm is simple and may serve as a reference for optimal design and operation of PEMFC.

Keywords: PEM fuel cell; Membrane electrode; Water balance; Optimization; Temperature control

Introduction

Proton Exchange Membrane Fuel Cells (PEMFC) directly convert chemical energy stored in H_2 into electrical energy through electrochemical reactions. They have attracted global attention due to advantages including high energy conversion efficiency, low noise, zero pollution, rapid startup, and high specific power. To meet automotive requirements for compact spaces and complex operating conditions, PEMFC performance, power density, and durability continue to improve while costs decline.

In November 2013, UK-based Intelligent Energy announced the highest automotive fuel cell power density achieved to date, reaching 3.7 kW/L volumetric power density and 2.5 kW/kg specific power density [1]. In 2014, Toyota launched the MIRAI fuel cell vehicle, achieving 3.1 kW/L and 2.0 kW/kg power density [2]. High-power operation generally requires increased back pressure to enhance reactant gas concentration, with current densities often reaching 1.0-2.0 A/cm^2. Consequently, substantial water is generated. If this product water can be properly utilized, the humidification system can be simplified, making pressurized operation with non-humidified cathodes and high current density a development trend [3,4].

When applied to vehicle power systems, control strategy is a critical factor determining efficient, durable, and stable operation. Optimized control strategies depend on effective identification of stack operating states, among which accurate identification of MEA water content is extremely important [5] yet exceptionally difficult.

Yuan [6], Jang [7], and Ding [8] explored optimal operating parameters including temperature, gas humidity, operating pressure, and flow field structure through simulation and experimental methods. Kanani [9] and Damour [10] proposed control models based on Response Surface Methodology and Flatness-based Approach to regulate operating conditions. Hu [11] and Cheng [12] utilized model-based methods to control MEA flooding state (via anode purge) and operating temperature, applying these to actual bus fuel cell systems. However, model accuracy—particularly the reliability of MEA flooding models—directly affects whether the system can operate efficiently and stably.

Shaul [13] proposed that operating PEMFC without external humidification, relying solely on product water to wet the proton exchange membrane, is feasible and established corresponding criteria. Janssen [14] experimentally investigated operating condition effects on net electro-osmotic drag coefficient, finding it largely independent of current density and nearly constant under cathode non-humidified, anode humidified conditions, with electrochemically produced water being almost entirely removed by cathode reactant gas. Based on this, Berning [15,16] explored ideal water balance under completely non-humidified conditions where outlet gases reach saturation, proposing control methods using cathode/anode outlet dew point temperature. However, they found such control achieves water balance but not optimal performance, with strict constraints on gas stoichiometry.

In light of these limitations, this paper addresses PEMFC operation at large current density with non-humidified cathode and pressurized anode/cathode. A zero-dimensional water balance model is established to obtain water balance temperature without net electro-osmotic drag under various back pressures and stoichiometries. Subsequently, considering small net drag coefficients, a corrected water balance temperature is derived. Finally, three-dimensional simulations accounting for electro-osmotic drag and liquid water effects are performed to modify the water balance temperature for optimal performance under corresponding operating conditions.

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1. Zero-Dimensional Water Transport Model in Fuel Cells

[Figure 1: see original paper] illustrates the water transport process in PEM fuel cells. Under steady-state conditions, water at cathode/anode inlet/outlet channels and reaction-generated water follow these relationships:

Cathode inlet water flow:

$$q_{w,c}^{in} = \frac{M_{H_2O}}{M_{air}} \cdot \frac{p_{sat}(T_{hum})}{p_{bp} - p_{sat}(T_{hum})} \cdot \frac{S_c}{r_{O_2}} \cdot \frac{i}{4F}$$

Anode inlet water flow:

$$q_{w,a}^{in} = \frac{M_{H_2O}}{M_{H_2}} \cdot \frac{p_{sat}(T_{hum})}{p_{bp} - p_{sat}(T_{hum})} \cdot S_a \cdot \frac{i}{2F}$$

Cathode outlet water flow:

$$q_{w,c}^{out} = \frac{M_{H_2O}}{M_{air}} \cdot \frac{p_{sat}(T_{cell})}{p_{bp} - p_{sat}(T_{cell})} \cdot \frac{S_c}{r_{O_2}} \cdot \frac{i}{4F}$$

Anode outlet water flow:

$$q_{w,a}^{out} = \frac{M_{H_2O}}{M_{H_2}} \cdot \frac{p_{sat}(T_{cell})}{p_{bp} - p_{sat}(T_{cell})} \cdot S_a \cdot \frac{i}{2F}$$

Defining positive direction as water flow from anode to cathode, the net electro-osmotic drag flux in the membrane is:

$$q_{mem} = n_d \cdot \frac{i}{F}$$

The water balance difference is:

$$\Delta q = q_{w,c}^{in} + q_{w,prod} - q_{w,c}^{out} - q_{mem}$$

Where $q_{w,prod} = \frac{i}{2F}$ is water generated in the cathode MEA; $q_{w,c}^{in}$ is cathode inlet water; $q_{w,a}^{in}$ is anode inlet water; $q_{w,c}^{out}$ is cathode outlet water; $q_{w,a}^{out}$ is anode outlet water; q_{mem} is net water flux through membrane; q_{back} is back-diffusion due to concentration gradient; q_{EOD} is electro-osmotic drag; q_{press} is pressure-driven diffusion; n_d is net electro-osmotic drag coefficient; d_{hum} is air humidity ratio; $p_{sat}(T)$ is saturated water vapor pressure at temperature T; p_{bp} is operating pressure; S_c is cathode air stoichiometry; S_a is anode hydrogen stoichiometry; M_{H_2O} is water molar mass (18 kg/kmol); M_{air} is air molar mass (28.8 kg/kmol); M_{H_2} is hydrogen molar mass (2 kg/kmol); r_{O_2} is oxygen volume fraction in air (typically 1/5); i is current density (A/cm^2); and F is Faraday constant (96487 C/mol).

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2. MEA Water Balance with Non-Humidified Cathode

For the operating conditions studied herein (non-humidified cathode gas), $q_{w,c}^{in} = 0$. Based on Janssen' s research, the total water flux through the membrane caused by electro-osmotic drag, back-diffusion, and pressure diffusion is much smaller than produced water [14]. Therefore, it is possible to remove all produced water via cathode gas to achieve saturated outlet conditions while ensuring no excess water accumulates in the MEA [13]. However, this water balance state tends to dry the membrane, resulting in suboptimal performance [15]. Optimal performance typically occurs when a small amount of liquid water exists on the cathode side, providing ideal membrane wetting [6]. This liquid water forms from condensation of generated and electro-osmotically dragged water, subsequently driven into flow channels by capillary pressure, making the cathode outlet gas supersaturated.

2.1 MEA Water Balance Without Net Electro-Osmotic Drag

Assuming zero net electro-osmotic drag between anode and cathode, the difference between generated water and cathode outlet water flow is defined as Δq:

$$\Delta q = q_{w,prod} - q_{w,c}^{out}$$

According to the Clausius-Clapeyron equation, the relationship between saturated water vapor pressure and temperature is [17]:

$$p_{sat}(T) = p_{atm} \cdot \exp\left(-\frac{\Delta H_{vap}}{R} \cdot \left(\frac{1}{T} - \frac{1}{T_{ref}}\right)\right)$$

[Figure 2: see original paper] and [Figure 3: see original paper] show Δq versus temperature and current density at cathode stoichiometry $S_c = 2.5$ and operating pressures of 200 kPa and 100 kPa, respectively. For a given pressure, Δq decreases with increasing temperature until reaching zero, then becomes negative with absolute value increasing with current density. The point where $\Delta q = 0$—where generated water is exactly removed by dry cathode gas reaching saturation at the outlet—is defined as the MEA water balance point, with corresponding temperature termed the water balance temperature. At 100 kPa, this temperature is 54.3°C; at 200 kPa, 69.59°C; and at 300 kPa, 79.33°C. Notably, the water balance temperature is independent of current density, depending only on pressure and stoichiometry. When operating temperature is below the balance point, Δq is positive, indicating excess water remains in the MEA as liquid, increasing with current density. When above the balance temperature, Δq is negative, requiring additional water that causes MEA dehydration. In actual operation, this additional water comes from humidification and anode electro-osmotic drag, with required amount increasing with current density.

[Figure 4: see original paper] shows Δq versus current density and operating pressure at $S_c = 2.5$ and $T_{cell} = 70$°C. Δq increases with pressure, indicating reduced water carrying capacity of gas and more residual water in the MEA. At 200 kPa, Δq is nearly zero and independent of current density, consistent with [Figure 2: see original paper] where the balance temperature is 69.59°C at 200 kPa.

[Figure 5: see original paper] demonstrates that water balance temperature increases with operating pressure but decreases with cathode stoichiometry. For a given pressure, increasing stoichiometry enhances gas water capacity without requiring temperature increase. Conversely, at fixed stoichiometry, increasing pressure reduces gas water capacity.

While this method simply obtains balance temperature under specific conditions, operating at this temperature dries the membrane, yielding non-optimal performance [15].

2.2 MEA Water Balance Considering Net Electro-Osmotic Drag

For typical PEMFC operation, cathode gas stoichiometry $S_c = 2.5–3$ and operating pressure $p_{bp} = 100–300$ kPa. The corresponding MEA water balance temperature variations are shown in [Figure 5: see original paper].

Under cathode non-humidified, anode humidified conditions, the net electro-osmotic drag coefficient $n_d \approx 0.2$ [14], meaning most water dragged from anode returns via back-diffusion. This is particularly true for the 15-µm Nafion membrane considered here, forming the theoretical basis for dew point temperature control. However, as noted, balance temperature control dries the membrane [15]. To achieve optimal wetting and performance, appropriate liquid water should exist in the MEA, requiring correction of the balance temperature in [Figure 5: see original paper].

Considering small net electro-osmotic drag and condensation effects, let q_{mem} be the net drag water flux. The balance equation becomes:

$$\Delta q = q_{w,prod} + q_{mem} - q_{w,c}^{out}$$

Based on Janssen [14], net drag coefficients of 0.05 and 0.1 are considered. [Figure 6: see original paper] shows Δq versus net drag coefficient at $S_c = 2.5$ and $p_{bp} = 300$ kPa. Since net drag is positive (water dragged from anode to cathode), higher temperatures are required to remove this extra water. The water balance temperatures become 81.36°C and 83.2°C for net drag coefficients of 0.05 and 0.1, respectively.

2.3 MEA Water Balance Based on Optimal Performance

The aforementioned dew-point-based MEA water balance temperature control (with positive net drag) tends to dry the proton exchange membrane, preventing optimal wetting and performance. Therefore, this study employs computational fluid dynamics software (Fluent) for three-dimensional simulations to determine the optimal operating temperature.

Main structural parameters and operating conditions are listed in . Due to space limitations, heat/mass transfer equations, electrochemical equations, and specific physical/electrochemical parameters are detailed in [6].

** Main Geometric Parameters and Operating Conditions**

Parameter	Value
Channel length; width; depth (mm)	50; 1.0; 0.4
Plate thickness (mm)	0.4
Membrane thickness; CL thickness; GDL thickness (mm)	0.015; 0.01; 0.2
Cathode gas stoichiometry S_c	2.5
Anode gas stoichiometry S_a	2.5
Operating pressure (absolute) p_{bp} (kPa)	100-300
Cell temperature T_{cell} (°C)	50-90
Cathode inlet relative humidity RH_c (%)	0
Anode inlet relative humidity RH_a (%)	50
Current density i (A/cm^2)	1.0-2.0

[Figure 7: see original paper] and [Figure 8: see original paper] show the optimal performance temperatures (dashed lines) obtained from simulation at $S_c = 2.5$ and back pressures of 100 kPa and 300 kPa, respectively. At 100 kPa, the water balance temperature is 54.3°C (current-density independent). While operation at this temperature allows generated water to be exactly removed with saturated outlet gas, the actual optimal operating temperature is approximately 47.7°C (slightly varying with current density). At this temperature, small amounts of liquid water form on the cathode side, but the membrane is well-hydrated. Considering oxygen transport and membrane conductivity, performance is optimal despite supersaturated cathode outlet gas. Operation below this temperature causes severe flooding; above it, the membrane gradually dries.

At 300 kPa, the performance zones are similar, though the optimal performance temperature and water balance temperature are much closer. At high back pressure, cathode gas water capacity decreases, so slightly lower temperatures provide adequate membrane wetting, consistent with [Figure 4: see original paper].

Berning et al. proposed using balance temperature for stack temperature control [14-16], but this dries the membrane regardless of net drag consideration. This study seeks optimal performance conditions based on existing mass transfer and electrochemical models, considering that: (1) current models are imperfect, potentially deviating from reality; (2) spatial temperature distribution within stacks is non-uniform, making single-point control impractical; (3) stack/MEA material and structural variations shift optimal performance lines; and (4) control system errors exist. Therefore, we propose maintaining operation within a high-performance region rather than strictly controlling to a calculated optimal line.

[Figure 9: see original paper] compares the simulation-corrected optimal performance temperature with the zero net drag water balance temperature at

$S_c = 2.5$. The optimal operating temperature is lower than the water balance temperature. This defines three operating zones: below optimal temperature (flooding), between optimal and balance temperatures (good performance), and above balance temperature (dry membrane). Actual temperature control can use the zero net drag balance temperature as a baseline plus a correction factor to maintain operation in the high-performance zone, providing a simple control algorithm.

Conclusions

This study investigated water transport and balance characteristics in PEMFC operating at large current density, proposing a temperature control method based on MEA water balance. Utilizing product water, the system employs non-humidified cathode, humidified anode (simulating recirculation humidification), and pressurized operation. Main conclusions are:

1. **For determined operating pressure and stoichiometry, a water balance temperature exists based on zero net electro-osmotic drag, independent of current density.** At this temperature, generated water is exactly removed by cathode outlet air. Operation above this temperature causes MEA dehydration; below it causes partial flooding. The balance temperature increases with back pressure and decreases with cathode gas stoichiometry.
2. **The zero net drag balance temperature algorithm is simple but yields dry membrane conditions** when used for temperature control, resulting in suboptimal performance.
3. **Three-dimensional simulation correction of the zero net drag balance temperature yields an operating temperature for optimal performance.** As operating pressure increases, the optimal performance temperature converges toward the zero net drag balance temperature. Operation at the optimal temperature line results in slight MEA flooding, but considering combined effects of membrane wetting and oxygen transport, the cell achieves best performance.
4. **Practical temperature control can use the zero net drag balance temperature as a baseline plus a correction factor** to maintain operation in the high-performance region, providing a simple control algorithm.

While the optimal performance temperature obtained through simulation may vary with MEA structure and material composition, the identified trends and temperature control methodology provide valuable reference for fuel cell design and operation optimization.

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Note: Figure translations are in progress. See original paper for figures.