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A real-time capable quasi-2D proton exchange membrane fuel cell model

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ABSTRACT

In this paper a dynamic proton exchange membrane fuel cell model for real-time applications is presented. Following a quasi-2D approach, effects such as multicomponent diffusion in porous layers, membrane water transport driven by diffusion and electro-osmotic drag as well as membrane nitrogen crossover forced by partial pressure differences, are considered. A linearisation of the governing equations with respect to the previous time step is applied to avoid numerically expensive Newton iterations and to speed up the simulation. Furthermore, a solution method based on Chebyshev collocation minimises the required number of nodes and assures real-time capability. The model is validated in terms of polarisation curves, current density and species distribution versus steady-state computational fluid dynamics simulations of a 3D fuel cell performed in AVL Fire™. The transient behaviour is found to be in good qualitative agreement with results published by other authors. Due to the fast computation capability of the presented model, it is suitable for widespread parameter studies, control unit adjustments or state predictions, e.g. fuel starvation or membrane drying and flooding.

Generally, bold faces and superscript tilde denotes vector and dimensional quantities, respectively.

1. Introduction

Proton exchange membrane fuel cells (PEMFCs) are a promising alternative power source for mobile and stationary devices. Low operating noise, the relative simplicity due to no moving parts, zero emission of greenhouse gases and a high energy density combined with high efficiency are the main advantages. In recent decades, fundamental knowledge about fuel cell (FC) operating conditions has been gained by studying both experimental and computer simulation results. However, dynamic operation of a FC is still very challenging and the issue of reduced durability and performance occurring from unmeant destructive states is hardly tackled successfully. State-of-the-art FCs are coupled to a battery to bridge dynamic load changes and achieve almost steady working conditions. Transient operation is of high interest for next generation FCs to avoid the battery's costs and weight. Therefore, real-time control will be essential to prevent local destructive states and maintain high efficiency. To this end, a FC model based on physical grounds is desirable for affordable testing, control unit adjustment, online monitoring and to perform widespread parameter studies with a minimum of computation time.

The first FC models were presented by Bernardi and Verbrugge [1] and Springer et al. [2] in the early 1990s. These models describe 1D mass transfer in the membrane direction and consider steady-state operation only. Springer et al. [2] introduced a model for the water transport across the membrane which partly is still used nowadays. A quasi-2D approach – coupling a 1D gas channel model with a 1D model for mass transport through the membrane electrode assembly – which is suitable to describe spatial variations of current density, water distribution and membrane ohmic resistance was presented by Dannenberg et al. [3]. This quasi-2D description was further used by many other authors [4–6]. While Berg et al. [4] presented a new approach to couple gas diffusion layers (GDLs) with the membrane considering non-equilibrium effects, Freunberger [5] and Kulikovsky [6] assumed equilibrium between the membrane water content and the GDL water vapour activity at the corresponding interface [2]. Similar to the quasi-2D approach, Tavčar and Katrašnik [7,8] presented a model designed for fast state prediction based on a quasi-3D computation domain, composed of a 1D model for the gas channels and a superimposed 2D model for the GDL and membrane assembly perpendicular to the gas channel flow direction. By assuming potential flow inside the GDL an analytical 2D solution, reducing the computational effort drastically, is

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Nomenclature

Latin symbols

$\tilde{a}_c\tilde{L}_c$	electrode roughness, meaning catalyst surface area per electrode geometric area [–]
a_w	water vapour activity [–]
C_{drag}	electro-osmotic drag coefficient in the membrane [–]
$\widetilde{\mathscr{D}}$	binary diffusion coefficient [m^2 s]
$\tilde{D}_H$	hydraulic diameter [m]
$\tilde{D}_w$	water diffusion coefficient in the membrane [$m^2\,s^{-1}$]
$\boldsymbol{e}_1$	unit vector in x_1-direction [–]
$\tilde{E}_{act}$	activation energy for O_2 reduction on platinum [J mol^{-1}]
$\tilde{E}_{cell}$	cell potential [V]
$\tilde{E}_{OC}$	open-circuit potential [V]
$\widetilde{EW}$	equivalent weight of the dry membrane [kg mol^{-1}]
$\tilde{F}$	Faraday constant, 96485.3365 C mol^{-1}
$f_{1,2}$	fitting parameters for PEM ionic conductivity [–]
F_c	hydraulic diameter correction factor [–]
f_D	Darcy-Weisbach friction factor [–]
F_u	shape factor [–]
$\tilde{H}$	height of channel, GDL, membrane [m]
$\tilde{i}$	reaction current density [A m^{-2}]
$\tilde{i}_0$	exchange current density [A m^{-2}]
$\tilde{j}$	diffusive species flux [kg $m^{-2}\,s^{-1}$]
$\tilde{j}^{tot}$	total species flux [kg $m^{-2}\,s^{-1}$]
K_{1-6}	dimensionless group [–]
K_e	dimensionless group [–]
$\tilde{k}_{N_2}$	nitrogen permeance in the PEM [mol (s m Pa)$^{-1}$]
$\tilde{L}$	PEMFC length [m]
$\widetilde{\mathscr{M}}$	molar mass [kg mol^{-1}]
$\tilde{p}$	pressure [Pa]
$\tilde{p}_{amb}$	ambient pressure [Pa]
$\tilde{p}^{sat}$	saturation pressure [Pa]
q	Bruggeman exponent [–]
$\tilde{R}$	universal gas constant, 8.314 J (mol K)$^{-1}$
RH	relative humidity at channel inlet [–]
$S_{m,u,s}$	source terms for conservation of mass, momentum and species, respectively
$\tilde{T}$	temperature [K]
$\tilde{T}_{cell}$	cell temperature [K]
$\tilde{t}$	time [s]
$\Delta\tilde{t}$	time step [s]
$\tilde{u}$	velocity [m s^{-1}]
$\tilde{u}_{in}$	inlet velocity [m s^{-1}]
$\tilde{u}_\alpha$	species velocity [m s^{-1}]
$\tilde{W}$	width of channel, GDL, membrane [m]

Greek symbols

α_c	catalyst layer transfer coefficient [–]
ε	gas phase volume fraction in porous media [–]
γ_c	pressure dependency factor for electrochemical reaction [–]
$\tilde{\kappa}_\perp$	through-plane hydraulic permeability [m^2]
$\tilde{\kappa}_\parallel$	in-plane hydraulic permeability [m^2]
λ	normalised membrane water content [–]
$\tilde{\mu}$	dynamic viscosity [Pa s]
$\tilde{\rho}$	density [kg m^{-3}]
$\tilde{\sigma}$	membrane ionic conductivity [S m^{-1}]
$\tilde{\tau}_w$	wall shear stress [N m^{-2}]
ξ	mass fraction [–]

Subscripts and superscripts

A	anode
C	cathode
r	reference value
T	transposed vector

Abbreviations

CFD	computational fluid dynamics
FC	fuel cell
GC	gas channel
GDL	gas diffusion layer
H_2	hydrogen
H_2O	water
LIT	linearisation in time
N_2	nitrogen
O_2	oxygen
PDE	partial differential equation
PEM	proton exchange membrane
PEMFC	proton exchange membrane fuel cell
SL	slice

obtained for the flow field. Even though the presented models highly improved the understanding of the FCs' behaviour, transient phenomena need to be considered for control applications.

A dynamic quasi-3D PEMFC model was presented by Kang [9], neglecting parallel diffusion fluxes in the GDL and the electrolyte, and using different numbers of control volumes to resolve mass and energy transport. The application of a two-phase water transport model through the GDL allowed to investigate the influence of liquid water formation on the FC's performance, by comparing the results of the two-phase model with those of a previously developed one-phase model. Gao and Bessler [10] proposed a transient 2D FC model, replacing Springer et al.'s piecewise form of the membrane water sorption isotherm by a continous expression and using transport equations in the channels and the GDLs. Their model also captures electrochemical kinetics of the oxygen reduction reaction and is, in a subsequent work [11], used for an electrochemical impedance analysis. Nyquist plots for different inlet gas humidities and membrane thicknesses are presented for co- and counter-flow configurations. Next to online monitoring, the investigation of varied impedance spectra may be of interest to enhance the FC's durability as it is a promising method for state of health observations. Another transient 2D PEMFC model following Springer's coupling approach and using pure oxygen (O_2) and hydrogen (H_2) as feed gases on cathode and anode side, respectively, was presented by Wu et al. [12]. They developed their work further to treat non-isothermal transient 3D-effects [13] and analysed the dynamic influence of Springer's equilibrium and Berg's non-equilibrium coupling methods between GDLs and the membrane. However, as their fuel cell is fed with pure O_2, phenomena related to the presence of nitrogen (N_2), as multicomponent diffusion, N_2 membrane crossover and material properties depending on the N_2 distribution have not been taken into account. Wang and Wang [14] presented a dynamical 3D model and studied the importance of various physical effects, such as membrane hydration, GDL species transport due to diffusion and convective gas transport in the gas channels, by considering the relevant time scales. The FC model is operated with humidified O_2 and H_2 and therefore only accounts for binary diffusion between fuel gas and water. Assuming isothermal cell conditions, transient simulations have been performed by using a commercial computational fluid dynamics (CFD) software. They analysed the dynamic response to step changes of cell potential and cathode inlet humidification. In their subsequent work [15], the model