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Modeling of the heat transfer in a portable PEFC system within MATLAB-Simulink

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Abstract

A dynamic model of a (portable) polymer electrolyte fuel cell system including the heat transfer between stack and periphery – here stack and metal hydride storage – has been developed within MATLAB-Simulink. The implemented equations describe the steady-state as well as the dynamic operation of the PEFC system with sufficient accuracy, although considerable simplifications have been made to keep model complexity and computing time low. As simulations are performed in 100-fold real time, different operating conditions and control strategies for PEFCs can be analyzed and evaluated in short-time. Here, emphasis is given to the operation limits of the PEFC system, i.e. the conditions for trouble-free operation at different loads and high or low ambient temperature are established. The model has been validated by experiments on a home-made portable system.

Keywords: PEFC; Model; Dynamic; Heat; System

1. Introduction

Fuel cells have progressed from the laboratory scale to market entrance in recent years [1]. Depending on the different requirements of the envisaged mobile, stationary or portable application, polymer electrolyte fuel cells (PEFC), solid oxide fuel cells (SOFC), molten carbonate (MC) or direct methanol fuel cells (DMFC) with different electrical power and heat output have been developed mainly by engineering skills. The possibility of design and performance improvement of fuel cell components (MEA, stack, etc.) and entire systems by simulation was recognized soon and several stationary [2–4] model descriptions have been elaborated. However, few dynamic simulations have been performed. Generally, they are based on a set of differential equations providing numerical solutions for the topic of interest. Saving expensive experiments and tests, such simulations are cost-effective and accelerate the fuel cell development considerably.

Concerning portable PEFC systems, the improvement of their (dynamic) behaviour at various operating conditions, including unfavourable ambient conditions (low/high T, fluctuating fuel supply), is a major task. Also the implemented components should be well balanced. Simulations are quite apt for both tasks and provide a decision basis for proper system design and optimal operation conditions.

In this paper a hydrogen operated PEFC system model implemented in MATLAB-Simulink is presented. Main goals of the model are:

1. to simulate the interactions between individual components
2. to serve as a tool for component design
3. to get decisive information for operation conditions
4. to predict dynamic behaviour of the entire system.

Special focus was placed on the thermal balance of the stack and a metal hydride cartridge in a small sized portable

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Nomenclature

A	area (m^2)
A_d	passed cross section (m^2)
A_m	area perpendicular to flow direction (m^2)
c_p	specific heat capacity ($J\,kg^{-1}\,K^{-1}$)
d	diameter (m)
E	voltage (V)
E^0	open cell voltage (V)
F	Faraday-constant ($C\,kmol^{-1}$)
ΔG	free reaction enthalpy ($J\,kmol^{-1}$)
h	height (M)
H	enthalpy ($J\,kmol^{-1}$)
ΔH	reaction enthalpy ($J\,kmol^{-1}$)
I	current (A)
l	length (m)
L	height of the plate (m)
L_0	characteristic length (m)
$\dot{m}$	mass stream ($kg\,s^{-1}$)
Nu	Nusselt number
P	power (W)
Pr	Prandtl number
$\dot{Q}$	heat flow (W)
R	universal gas constant ($J\,kmol^{-1}\,K^{-1}$)
Ra	Rayleigh number
Re	Reynolds number
ΔS	reaction entropy ($J\,kmol^{-1}\,K^{-1}$)
t	time (s)
T_c	critical temperature (K)
U	circumference (m)
V	velocity ($m\,s^{-1}$)
w_0	reference velocity ($m\,s^{-1}$)

Greek symbols

α	heat transfer coefficient ($W\,m^{-2}\,K^{-1}$)
ζ	adjustment factor
Δ	difference
η	dynamic viscosity ($kg\,m^{-1}\,s^{-1}$)
ϑ	temperature (°C)
λ	heat conductivity ($W\,m^{-1}\,K^{-1}$)
ν	kinematic viscosity ($m^2\,s^{-1}$)
ρ	density ($kg\,m^{-2}$)
Ω	ohmic resistance (Ω)

Subscripts

a	anode
c	cathode
cart	cartridge
corr	corrected
el	electric
fcreac	fuel cell reaction
foconv	forced convection
frconv	free convection
F	fluid
h	hydraulic
lam	laminar
m	averaged
reac	reaction
rib	cooling fin
th	thermal
tur	turbulent
W	wall
0	state at the position y = 0
∞	infinity

PEFC system (power of about 200 W) in order to optimize the thermal balance of these components, as these are often the critical components in the system set-up (note that these two components have complementary characteristics, the stack acting as heat source and the hydride as heat sink). The requirement of real time operation led to a simplified one-dimensional dynamic stack model and a zero-dimensional model of the auxiliary components. As shown in the following, the developed model describes the dynamic properties of a PEFC system satisfactorily and can be readily employed in the optimization and real time control of PEFCs.

2. System modeling approach

In this study a comprehensive PEFC system model was developed to investigate the energy as well as the mass dynamic interactions between the implemented components. A very flexible structure arises by modeling the components as different autonomous operating blocks, see Fig. 1.

The air for the cathode reduction reaction is supplied by a compressor which controls the pressure and flow rate. The hydrogen for the oxidation at the anode side of the fuel cell is

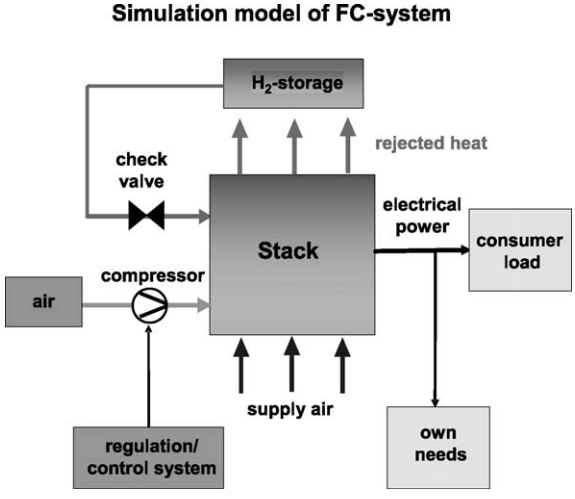

Fig. 1. Model of H_2 PEFC system including thermal coupling between stack and hydrogen storage.

provided by a metal hydride storage, whereas the pressure is controlled by a check valve. The hydride storage is coupled to the stack via the cooling cycle, i.e. the hydride cartridge temperature is controlled by the air passing the stack. This set-up was chosen to prevent insufficient hydrogen supply at high power levels or low temperature as the desorption reaction of hydrogen from metal hydride is endothermal and the desorption pressure is a function of the temperature. Furthermore, a control system was added in order to test different operation strategies. In the following the main components and the coupling between stack and metal hydride cartridges are considered in more detail.

2.1. PEFC stack model

Concerning the stack model the assumption is made that it consist of 20 single cells having identical behaviour (this number arises from the stack used in the experimental part). This is corresponding to a parallel supply of single cells, which do not affect each other and leads to a homogeneous temperature distribution across the stack in all directions in space. The most important input and output parameters of the stack are listed in Table 1. The various energy values arise by a multiplication of the single cell values with the number of cells contained by the stack.

For the description of the single cell a one-dimensional dynamic model was elaborated. Herein the cell is divided into seven control volumes, each considering the specific physical and electrochemical characteristics. In terms of the diffusion and the catalyst layer mass balances for existing species hydrogen, nitrogen, oxygen, water vapour and liquid water are accomplished using the material transport equations from ref. [5]. As regards the membrane part, the effects of concentration gradients and the electro-osmotic drag for water transport through the membrane are incorporated [2]. Having determined the partial pressures of the gaseous species, the water amount in the different layers, the polarization losses at anode and cathode and the membrane voltage loss can be calculated. In case of the electrodes the polarization losses are computed by taking the double layer capacity into account. The output of the model is the single cell voltage, the electrical and thermal energy. As this paper is especially focused on the thermal coupling between stack and metal hydride storage, more detailed information and a model validation is given in [6]. Only the various equations necessary for our case are presented below.

Table 1
Important parameters of stack model

	Stack
Constants	Cell area Number of cells in the stack Heat capacity Gas volume anode Gas volume cathode Initial conditions (temperature, gas compositions, pressure)
Input parameters	Load current/power Cooling medium (type, temperature, flow rate) Gas inlet (pressure, flow rate, temperature, composition)
Output parameters	Voltage/current Cooling medium (temperature) Gas outlet (pressure, flow rate, temperature, composition)

2.1.1. Cell voltage and energy equations

The equilibrium potential E^0 for the cell can be derived from Nernst equation (Eq. (1)) and is a function of pressure and temperature

$$E^0 = -\frac{\Delta G^\circ}{nF} + \frac{\Delta S}{nF}(T - T^0) + \frac{RT}{nF}\left[\ln\frac{p_{H_2}}{p^0} + \frac{1}{n}\ln\frac{p_{O_2}}{p^0}\right] \quad (1)$$

Under current generation voltage losses on the anode (E_a) and cathode side (E_k) occur, depending on the chemical reaction, the double layer resistances and transport limitations [7]. In addition the potential is lowered by the ionic conductivity of the membrane and the electronic conductivity of bipolar plates (E_Ω). The resulting cell voltage is given by

$$E_{cell} = E^0 - E_a - E_k - E_\Omega \quad (2)$$

Hence, the electric power can be calculated from the cell voltage loss by

$$P_{el} = E_{cell} I \quad (3)$$

The emitted thermal power can then be calculated from the potential deviation against the equilibrium potential

$$P_{th} = (E_0 - E_{cell}) I \quad (4)$$

2.2. Compressor

In terms of the compressor a set of curves containing the flow rate and the pressure at the outlet have been established which are depending on the accepted current. Furthermore the rise of temperature associated with the compression of the air was implemented. The input and output parameters of this system component are listed in Table 2.

2.3. Metal hydride cartridges

Due to their convenient handling and safety properties metal hydrides are commonly considered as useful medium

Table 2
Input and output parameters of the compressor block

Parameters	Compressor
Input	Load current
Output	Flow rate pressure at outlet gas temperature

for the hydrogen storage in portable PEFCs. The desorption reaction of hydrogen is incorporated into the model via the enthalpy form of the energy equation which allows to calculate the anode pressure via the van't Hoff diagram of the metal alloy used. In order to provide secure operation of the stack a minimal inlet anode pressure of 1.5 bar_{abs} has to be ensured in our case. This requirement leads to a minimal operating temperature of −5 °C.

2.4. Thermal equations

For the thermal energy balance of the PEFC system three control volumes, namely stack, cooling medium and hydride storage, were adopted. Concerning the stack the thermal balance contains the fuel cell reaction as source; sinks are the forced convective heat transfer by means of the cooling medium and the free convective heat transfer to the surrounding air. In terms of the metal hydride cartridges, the heat transfer from the cooling medium and the thermal energy needed for the desorption reaction are balanced. The corresponding equations implemented in the model are given in the further sections.

2.4.1. Thermal conductance

All thermal-conducting processes can be described using the Fourier law [8]. For a one-dimensional approach the general equation can be reduced to the following equation:

$$\dot{Q} = \alpha A_m(\vartheta_W - \vartheta_F) \tag{5}$$

In order to solve this equation the knowledge of the heat transfer coefficient is necessary which can either be derived from partial differential equations or by using the theory of dimensionless operating figures [8,9]. In this work the latter is used in order to reduce the model complexity. The most important of these figures are the Nusselt, the Reynolds and the Prandtl number

$$Nu := \frac{\alpha L_0}{\lambda} \tag{6}$$

$$Re := \frac{\omega_0 \rho L_0}{\eta} \tag{7}$$

$$Pr := \frac{\eta c_p}{\lambda} \tag{8}$$

2.4.2. Thermal balance around the stack

With respect to the free convective heat transfer from the end plates of the stack to the surrounding air, the Nusselt number can be computed using the empirical equation (Eq. (9)) derived by Churchil and Chu for a vertical plate [8–10]. Herein the characteristic length required for computation is determined by the height of the plate

$$Nu = \left\{ 0.825 + \frac{0.387 Ra^{1/6}}{[1 + (0.492/Pr)^{9/16}]^{8/27}} \right\}^2 \tag{9}$$

The required Rayleigh number is given by the following equation:

$$Ra = \frac{\beta_\infty(\vartheta_0 - \vartheta_\infty) g L^3}{v^2} Pr \tag{10}$$

To calculate the heat transfer from the cooling fins of the stack to the flowing medium (air) we adopt a square channel geometry. For the forced convective heat transfer three different cases depending on the flow conditions of the cooling medium have to be distinguished [8–10]. In terms of a turbulent stream ($Re > 100{,}000$) the following equation is valid:

$$Nu_{tur} = \frac{\zeta/8(Re - 1000)Pr}{1 + 12.7\sqrt{\zeta/8}(Pr^{2/3} - 1)} \left[1 + \left(\frac{d_h}{L} \right)^{2/3} \right] \tag{11}$$

ζ can be determined by means of the following equation:

$$\zeta = \frac{1}{(1.82 \log_{10}(Re) - 1.64)^2} \tag{12}$$

If the Reynolds number is lower than 2300 the stream is laminar and the following equation can be used for the computation:

$$Nu_{lam} = \left\{ 3.66^3 + 0.7^3 + \left[1.615 \left(Re\, Pr \frac{d_h}{L} \right)^{1/3} - 0.7 \right]^3 \right\}^{1/3} \tag{13}$$

The hydraulic diameter required for the Reynolds number results from the following equation:

$$d_h = 4 \frac{A_d}{U} \tag{14}$$

In the transition region ($2300 < Re < 10{,}000$) both fractions are weighted using the following equation:

$$Nu = (1 - g) Nu_{lam} + g Nu_{turbulent} \tag{15}$$

The temperature of the stack can be calculated using the following equation:

$$\frac{d\vartheta_{stack}}{dt} = \frac{\dot{Q}_{fcreac} - \dot{Q}_{frconv} - \dot{Q}_{foconv}}{\rho_{stack} c_{pstack}} \tag{16}$$

2.4.3. Thermal balance around metal hydride cartridges

The thermal coupling between the flowing air and a cylindrical hydride cartridge can be modeled as a cylinder in a square channel circulated longitudinal by the fluid. The square channel can be further reduced to a coextensive tube, corresponding to heat transfer in an annular gap. Laminar and turbulent flow have to be differentiated again. In case of laminar flow Eqs. (17)–(19) are valid

$$Nu_{lam} = \left\{ Nu_{corr} + \left[f \frac{0.19(Re\, Pr\, d_h/L)^{0.8}}{1 + 0.117(Re\, Pr\, d_h/L)^{0.467}} \right] \right\} \times \left(\frac{\vartheta_m}{\vartheta_W} \right)^{0.12} \tag{17}$$

with the corrected Nusselt number Nu_{corr}

$$Nu_{corr} = 3.66 + 1.2\left(\frac{d_i}{d_a}\right)^{-0.8} \quad (18)$$

and the form factor given by

$$f = 1 + 0.14\sqrt{\left(\frac{d_a}{d_i}\right)} \quad (19)$$

If turbulent flow is existent ($Re > 2300$), the subsequent equations based on the Prandtl–Taylor-analogy [7] are valid

$$Nu = Nu_{corr}0.86\left(\frac{d_a}{d_i}\right)^{0.16} \quad (20)$$

with the corrected Nusselt number Nu_{corr}

$$Nu_{corr} = \left[\frac{(z/8)(Re - 1000)Pr}{1 + 12.7\sqrt{(z/8)}(Pr^{2/3} - 1)}\right]\left[1 + \left(\frac{d_a}{L}\right)^{2/3}\right] \times \left(\frac{\vartheta_m}{\vartheta_W}\right)^{0.12} \quad (21)$$

and

$$z = [1.82(\log_{10}(Re)) - 1.64]^{-2} \quad (22)$$

By means of these equations the heat flow from the surrounding medium to the cartridge can be computed. With the knowledge of the heat required for the desorption reaction, the temperature of the cartridge can then be calculated by integrating the following:

$$\frac{d\vartheta_{cart}}{dt} = \frac{\dot{Q}_{cart} - \dot{Q}_{reac}}{\rho_{cart}c_{pcart}} \quad (23)$$

3. Simulation results, validation and discussion

In order to validate the heat transfer model, the temperature gradients of the stack, of the cooling medium and of the metal hydride cartridge obtained by the simulation are compared with experimental results on the PEFC system mentioned above. The system configuration and the various temperature measurement positions in the experimental set-up are displayed in Fig. 2.

The validation of the model was accomplished with respect to steady state and dynamic system behavior. In the first case the load current was suddenly enhanced from 0 to 12 A (maximum current in applications) and kept constant until the temperature of the stack reached an upper limit. The temperature of the cooling medium was adjusted to 22 °C (=simulation boundary conditions). The further parameters used are listed in Table 3. In Fig. 3 the results obtained from both experimental and simulation are depicted.

As can be seen from the diagram, the stack temperature increases with time and approximates to an upper limit where the balance between thermal energy produced by the reaction and thermal energy transferred to the cooling media is achieved. Under the given geometry this upper limit especially depends on the flow rate of the cooling medium (adjustable by varying the fan power). The temperature change within the first time period is mainly defined by the heat capacity of the stack and the load applied. If the load is taken off an opposite temperature profile is obtained. The temperature change of the metal hydride cartridge is also given in Fig. 3 and shows complementary behaviour to

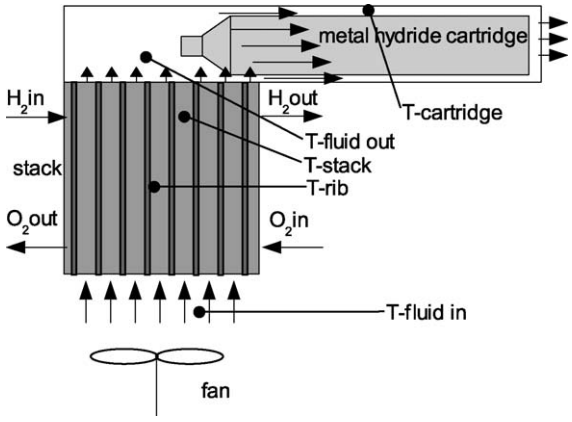

Fig. 2. Experimental system configuration with temperature measurement positions in the experimental set-up used for model validation.

Table 3
Boundary conditions/set of parameters for simulation of an equilibrium condition

V_{air}	0.006 $m^3 s^{-1}$
$d_{cartridge}$	0.05 m
$l_{cartridge}$	0.33 m
$l_{channel}$	0.33 m
$d_{a\ channel}$	0.06 m
Number of cartridges	2

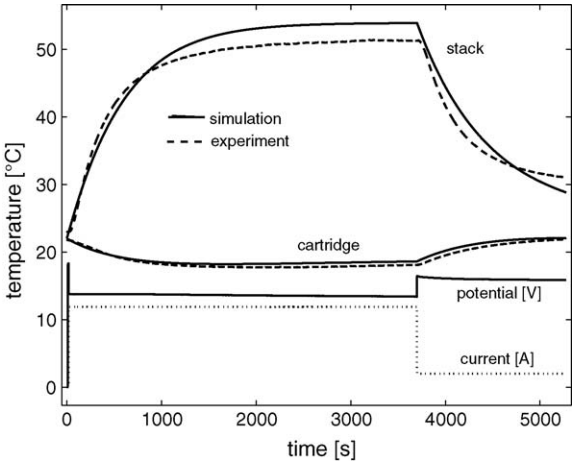

Fig. 3. Temperature characteristics of stack and metal hydride cartridges at an ambient air temperature of 20 °C and a load current of 12 A.

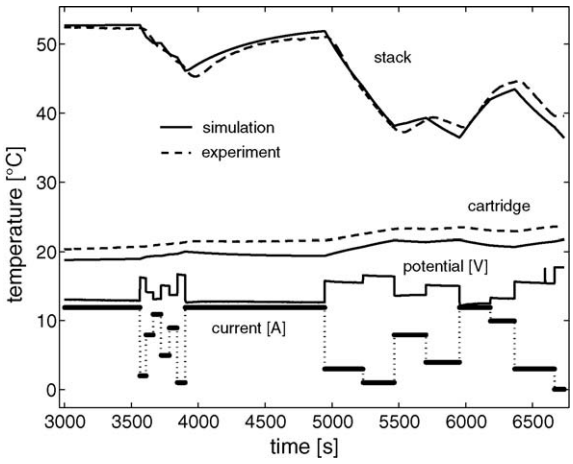

Fig. 4. Dynamic temperature characteristics of stack and metal hydride cartridges at an ambient air temperature of 20 °C and varying current.

the stack profile. In the beginning the temperature slightly decreases because of the endothermal hydrogen desorption reaction. With increasing temperature of the stack the transmitted thermal energy to the cartridges increases by means of the thermal coupling. The slope of the temperature curve changes its sign when the equilibrium between thermal energy needed for the reaction and the thermal energy transferred to the cartridges is reached. From the good agreement between simulation data and experimental results it can be concluded that the equations implemented in the model describe the real system correctly. The observed deviations are all in the range of measurement uncertainties.

The model also describes the dynamic behaviour of the PEFC system with sufficient accuracy as can be seen from Fig. 4 where random loads or potential steps, respectively, of different height have been investigated. Evidently the simplifications made in the model cause only minor, acceptable deviations. Once validated by experiment, the model can be used to identify critical system conditions, e.g. overheating of the stack at elevated ambient temperature. In the following sections different operating states are simulated to demonstrate the quality of the model. Fig. 5a shows the stack temperature change with increasing load at system start-up at 40 °C. According to the predicted temperature characteristics it appears advisable to limit the power output of the stack to avoid operation beyond the critical temperature for long time operation (here 60 °C). The maximum current from the stack under this conditions is limited to 10 A (corresponding to a distinct reduction in available power). Operating states at higher currents can only be maintained for short-time periods. At lower currents the operation is, of course, feasible over longer time periods. Fig. 5b presents the simulation results of the dynamical operation mode. Herein the time periods where high currents are demanded from the system have been restricted in such a way that the temperature cannot exceed the upper limit. Stated differently, the simulation results provide important parameters for secure system operation. Reduction of the power output may be a reasonable choice for short periods of operation at unfavourable conditions, or may be tolerable if the restricted power is sufficient for all situations. Installation of an extra cooling fan and, more elegantly, use of hybrid systems with supercaps as power sources on demand have to be considered, however, to achieve progress.

As in the case of operation at elevated ambient temperature, PEFC systems with metal hydride storage have deficiencies at low temperatures. In our case the pressure at the hydride storage reaches the critical value for trouble-free operation at about −5 °C. Therefore, system simulations at low T (close or equivalent to zero) have been accomplished. The resulting temperature curves are depicted in Fig. 6. In these simulations the initial conditions for ambient temperature and stack temperature have been set to 1 °C (the equations implemented in the stack model are only valid for temperatures higher than 0 °C).

In case of low currents, the temperature of the hydride cartridge decreases only slightly to below 0 °C, since the

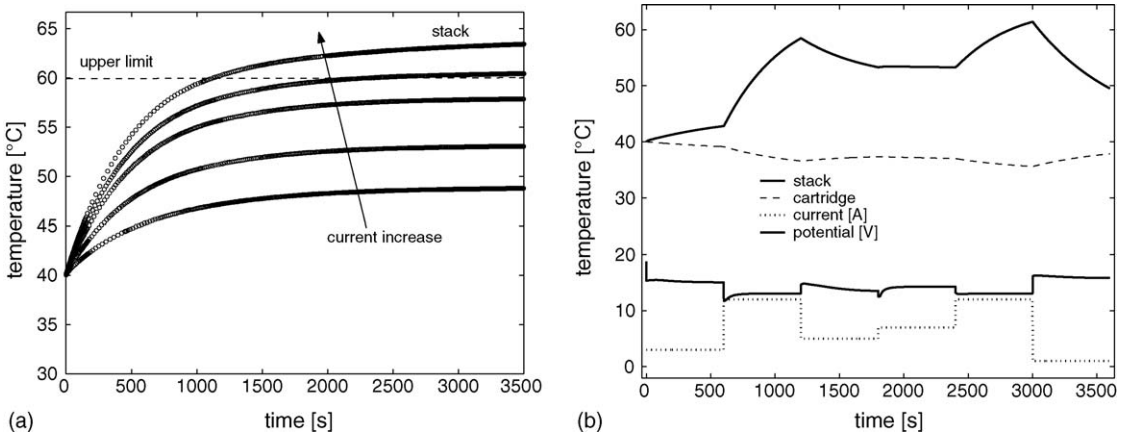

Fig. 5. (a) Temperature profiles of stack at different currents 5, 7, 9, 10 and 11 A and ambient temperature of 40 °C. (b) Dynamic variation of the current at an ambient temperature of 40 °C.

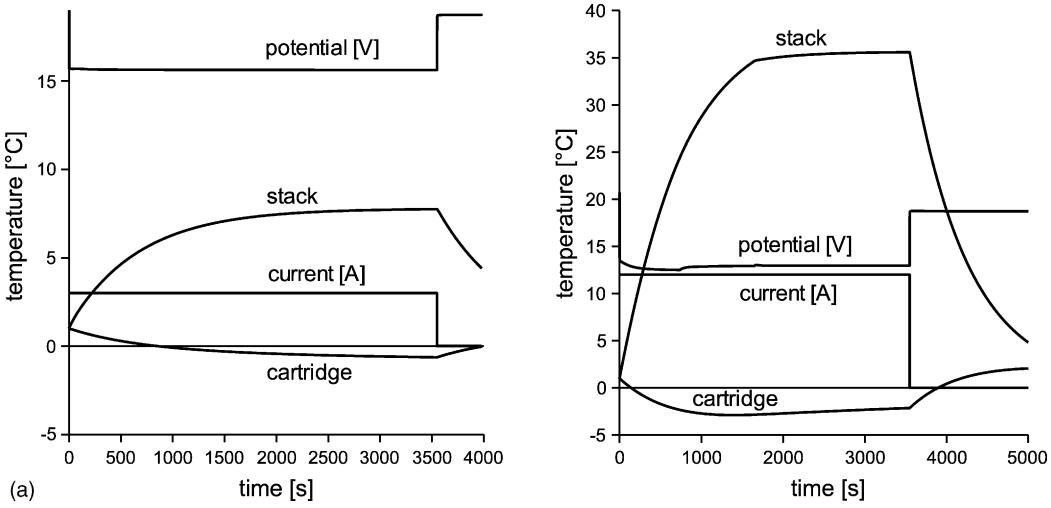

Fig. 6. (a) Temperature profile of stack and metal hydride cartridge at load current alternation from 0 to 3 A and an ambient temperature of 1 °C. (b) Temperature profile of stack and metal hydride storage at a load current alternation from 0 to 12 A and an ambient temperature of 1 °C.

H_2 desorption rate and therefore the energy needed for the endothermal reaction is low. At these operating conditions no critical state is reached as the thermal energy transferred from the stack to the cooling medium is always sufficient to balance the thermal energy needed for the desorption reaction of hydrogen. Even at a current of 12 A, where the hydrogen desorption rate is high, the storage temperature does not fall below −5 °C. This is a major advantage of the coupling between the cooling medium and the cartridge. As in the high temperature case simulations prove to be helpful for system optimization, allowing uninterrupted operation at extreme conditions.

4. Conclusions

A dynamic model for polymer electrolyte fuel cell systems has been derived and implemented within MATLAB-Simulink as modeling environment. Different autonomous working blocks are linked within the graphical user interface, each representing an essential system component. Within these blocks the properties are modeled using either common physical and thermodynamical equations or a curve family. In this work the model is primarily used to calculate the heat transfer between system components, notably stack-hydride storage, often realized in portable PEFC systems. For this purpose the general Fourier law, reduced to the one-dimensional case, and the similarity theory are considered to calculate the heat flow between the linked components. As validated by experiment, the implemented equations describe the steady-state and also the dynamic operation states sufficiently well, although considerable simplifications have been made to keep complexity and computing time low.

To demonstrate the capability of the model, different operating conditions have been simulated. Main emphasis has been laid on the modeling of extreme conditions, especially high and low temperature PEFC operation. Unfavourable conditions have been identified at which the stack temperature exceeds the limit given by the stack manufacturer. Similarly, operation near zero has been analyzed. As predicted by the simulations and verified by experiment, the thermal coupling between stack and hydride storage leads to trouble-free operation at temperatures close to zero for all load currents. The presented model can be used to ascertain whether different components fit the requirements for a stable handling by means of the modular construction. In addition it can serve as decision basis for different operating conditions and to estimate the interaction between the different components as simulations are performed in 100-fold real time. Beyond this, the model will be very useful to develop control strategies for secure operation. Extension of the study to hybrid systems is planned.

References

[1] P. Costamagna, S. Srinivasan, Quantum jumps in the PEMFC science and technology from the 1960s to the year. Part II. Engineering, technology development and applications aspects, J. Power Sources 102 (2001) 253–269.
[2] D. Benardi, W. Verbrugge, A Mathematical model of the solid–polymer–electrolyte fuel cell, J. Electrochem. Soc. 139 (1992) 2477–2491.
[3] S. Um, C.Y. Wang, Three-dimensional analysis of transport and electrochemical reactions in PEFCs, J. Power Sources 125 (2004) 40–51.
[4] D. Natarajan, T. Van Nguyen, A two-dimensional, two-Phase, multicomponent, transient model for the cathode of a PEFC using conventional gas distributors, J. Electrochem. Soc. 148 (2001) A1324–A1335.
[5] C. Rieckmann, Lösung des Problems der Diffusion und Reaktion in dreidimensionalen Porennetzwerken fur allgemeine Kinetiken, Ph.D. theses, TU Hamburg-Harburg, 1997.

[6] Z. Lemeš, A. Vath, Th. Hartkopf, H. Mäncher, Dynamic fuel cell models and their application in hardware in the loop simulation, J. Power Sources, in press.
[7] C.H. Hamann, W. Vielstich, Elektochemie, 3.Auflage, Wiley-VCH, 1998.
[8] H.D. Baehr, K. Stephan, Wärme- und Stoffübertragung, 3.Auflage, Springer-Verlag, 1998.
[9] F.P. Incropera, D.P. DeWitt, Fundamentals of Heat and Mass Transfer, 4th ed., Wiley-VCH, 1996.
[10] Verband Deutscher Ingenieure, Wärmeatlas, 7.Auflage, 1994.