CONTRIBUTION TO MODELING OF HYDROGEN PEM FUEL CELLS THERMAL PROCESSES

Matej Barát, Michal Stromko, Viktor Ferencey

Abstract:

This contribution deals with thermal modeling and simulations of the air-cooled PEM (Proton Exchange Membrane) fuel cell for power systems of transportation applications. PEM fuel cell is an electrochemical energy conversion device which converts chemical energy of hydrogen and oxygen directly and efficiently into electrical energy with waste heat and liquid water as by-products of the reaction. There is a number of advantages to a PEM fuel cell powered electromobiles that use hydrogen such as energy efficient and environmentally benign low temperature operation, quick start-up, compatibility with renewable energy sources and ability to obtain a power density competitive with the internal combustion engine in the perspective. Thermal analysis and thermal modeling of the air-cooled fuel cells are, however, a major problems that stems from a low operating temperatures of PEM fuel cell stacks in contrast to the conventional internal combustion engines. In the present study, a numerical thermal model is presented in order to analyse the heat transfer and predict the temperature distribution in air-cooled PEM fuel cells. In order to validate the performance of the created analytical simulation model, comparisons of the data obtained through experimental measurements in the Fuel Cells laboratory have been made.

Keywords:

PEM fuel cells, Power system, Thermal engineering, Temperature, Heat transfer, Air cooling, Hydrogen fuel, Electrochemical device, Conversion, Temperature distribution.

ACM Computing Classification System:

Hardware, Power and energy, Thermal issues, Energy generation and storage.

Introduction

The Proton Exchange Membrane Fuel Cell (PEM FC) is very flexible in terms of its power and capacity requirements, its long-life service, good ecological balance and very low self-discharges [1].

PEMFC offers high power density, quick start-up and low operating temperatures as well as rapid response to varying operational loads in many applications [2]. Currently, a PEM FC with a net power density of 1kW/L has been achieved [4].

Air-cooled proton exchange membrane fuel cells (PEM FCs), combining air cooling and oxidant supply channels, offer a significantly reduced bill of materials and system complexity compared to the conventional, water-cooled fuel cells. In air-cooled PEM FC systems, ambient air is applied freely as the cooling medium which means that the cooling environment is highly influenced by the ambient temperature. High inlet air temperature would reduce the cooling efficiency.

Air-cooled fuel cell systems combine the cooling function with the cathode flow field and reduce overall cost by eliminating a lot of auxiliary systems required for conventional fuel cell designs (water cooling loop, air compressor and humidifier) [4].

Operation of a proton exchange membrane fuel cell (PEM FC) is a complex process that includes electrochemical reactions coupled with transport of mass, momentum, energy and electricity [5].

The operating conditions for the best performance require a balance between temperature, humidity and reactant flow rates in order to avoid flooding of electrodes [6]. The sensitivity of PEM fuel cell stacks to temperature is mainly related to the required moisture levels in the membrane that is hydrated from water back-diffusion flux from the cathode to the anode. When the operating current density increases, the effects of temperature on membrane hydration decrease slightly.

However, heat is also needed for improved reaction kinetics at the catalyst layers. The effects of the heat to the operation of a fuel cell are subjective and complex. Heat is needed to improve the reaction kinetics, but too much heat would lead to an increase in energy losses [7]. Therefore, thermal management of PEM fuel cells needs to balance delicately with both requirements.

The Proton Exchange Membrane Fuel Cell (PEM FC) is very flexible in terms of power and capacity requirements, its long-life service, good ecological balance and very low self-discharges [4].

Temperature is a crucial parameter for PEM fuel cell performance which directly or indirectly affects the reaction kinetics, transport of water, humidity level, conductivity of membrane, catalyst tolerance, removal of heat or thermal stresses in the membrane etc. [4].

To conclude, the performance of the fuel cell increases as the temperature increases from room temperature to 80°C, further increase in temperature results in a current density dependent performance. The best performance was observed at around 80°C with 3 bars of absolute back pressure and 100% relative humidity.

For small size and performance of stacks (below 100W), the cooling can be achieved only with cathode air flow. A disadvantage here is that it requires relatively bigger channel size for cathode side of the stack compared with the anode side which consequently increases the volume of the stack. Stacks bigger than few hundred watts require a separate cooling channels.

1 Heat Sources in PEM FC

The electrical performance of a PEM fuel cell dictates the generated thermal energy within the stack. The theoretical power curve of a fuel cell can be obtained by establishing electrochemical models based on the Nernst equation and subsequent voltage losses within the stack. Higher voltage losses at a specified current density lead to a higher heat generation. During the operation of a PEM FC, hydrogen molecules are supplied at the anode and split into protons and electrons. The polymeric membrane conducts protons to the cathode while the electrons move from anode to cathode through an external load powered by the cell. Oxygen (from air) reacts with the protons and electrons in the cathode half-cell where water and heat are produced.

The overall reaction of a PEM fuel cell is: $\mathbf{H_2 + ½\ O_2 > H_2O}$ **+ electrical energy + heat energy**

1.1 Heat Generation

All the chemical energy that we have available in a fuel cannot be converted into useful work (electrical energy) because of the enthalpy (entropy) change during a chemical reaction. The heat generated within fuel cells is assumed to be the heat generated mainly at the electrochemical reaction sites of the cathodes. Generally, to determine the amount of heat produced by a fuel cell, an energy balance for a fuel cell stack can be provided:

$$\sum_i H_{i,in} = \sum_i H_{i,out} + P_{el} + \dot{Q}_{gen}, \quad (1)$$

or:

$$\dot{Q}_{gen} - \Delta H_i + P_{el} = 0, \quad (2)$$

where: $H_{i,in}, H_{i,out}$ are the enthalpies of reactants and products [kJ/kmol], P_{el} is the electrical power generated by the fuel cell [W], $\dot{Q}_{gen}$ is heat generated by the fuel cell, [W].

The amount of heat generated can be estimated using the simplified relations based on the energy balance of the system and depending on the state of water formed [7]:

$$\frac{I_{FC}}{nF} H_u n_{cell} = I_{FC} E_{cell} n_{cell} + \dot{Q}_{gen}, \quad (3)$$

where: H_u is low heating value of hydrogen [kJ/kg].

If the water exists as vapor at room temperature, then the E_{Nernst} voltage is 1.254 [V] and the stack thermal power P_{th} is dependent on the current produced and cell voltage [6]:

$$\dot{Q}_{gen} = P_{th} = (E_{Nernst} - E_{cell}) I_{FC} n_{cell} \quad (4)$$

A fuel cell stack may dissipate its heat energy by internal as well as external mechanisms. Internal heat removal by the cathode fluid stream is more significant than the anode fluid stream as the exothermic reactions occur at the cathode and produced water absorbs the generated heat.

A simple way to improve the performance of a fuel cell is to operate the system at its maximum allowed temperature. At higher-temperature, the electrochemical activities increase, and the reaction takes place at a higher rate, which in turn increases the power output. On the other hand, operating temperature affects the maximum theoretical voltage at which a fuel cell can operate. Higher temperature corresponds to lower theoretical maximum voltage and lower theoretical efficiency. Temperature in the cell also influences cell humidity which significantly influences membrane ionic conductivity. Therefore, temperature has an indirect effect on the cell performance through its impact on the membrane water content. The durability of the membrane electrolyte is another barrier for higher-temperature operation due to performance degradation during long-term operation. Scientists analyzed electrochemical performances as a function of the temperature distribution.

2 Analytical Simulation Model of PEM FC Stack

From the governing equations discussed before, an analytical zero-dimensional dynamic simulation model was created in Matlab Simulink environment. Topological diagram of the created simulation model can be seen in (Fig.1). The model consists of three interconnected subsystems which are responsible for simulating electrochemical, thermodynamic and mass transport effects that occur within the fuel cell stack. With this model, it's possible to analyze the effects of ambient and operating conditions on generated output power of the used fuel cell stack in steady state and transient modes of operation [8], [11].

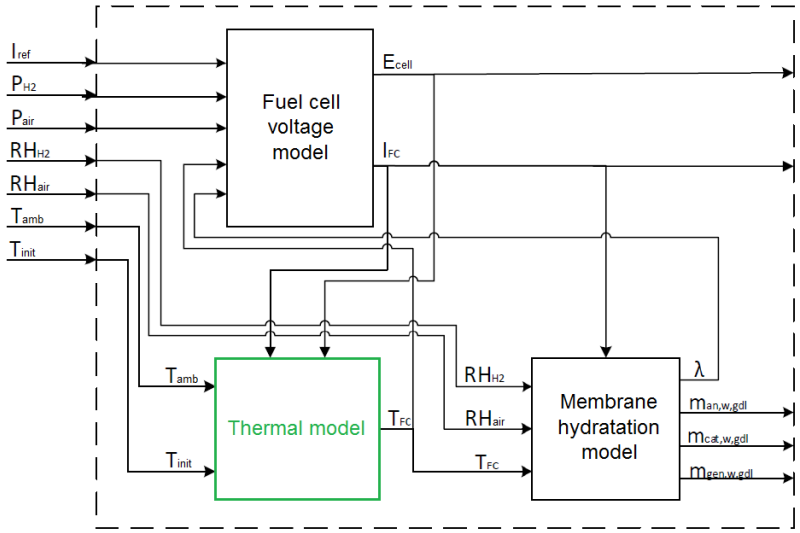

Fig.1. Topological diagram of PEM FC analytical model [8],[11].

Input parameters of the model:

I_{ref}	– load current (reference current) [A]
P_{H2}	– pressure of the hydrogen [atm]
P_{air}	– pressure of the ambient air [atm]
RH_{H2}	– relative humidity of the hydrogen [%]
RH_{air}	– relative humidity of the ambient air [%]
T_{amb}	– temperature of the ambient air [°C]
T_{init}	– initial temperature of the FCS [°C]

Output parameters of the model:

E_{cell}	– generated voltage of the fuel cell [V]
I_{FC}	– generated current of the fuel cell [A]
$m_{an,w,gdl}$	– amount of water transferred from membrane to anode GDL [l]
$m_{cat,w,gdl}$	– amount of water transferred from membrane to cathode GDL [l]
$m_{gen,w,gdl}$	– total amount of generated water [l]

Internal parameters of the model:

λ	– relative water content in the membrane [-]
T_{FC}	– actual working temperature of the FC [°C]

The focus of this paper is the thermal analysis of the PEM FC and therefore, the thermal subsystem highlighted with green color in the (Fig.1) will be further discussed in detail.

2.1 Thermal Model of PEM FC Stack

The thermal model of PEM fuel cell stack describes the changes of stack temperature depending on the ambient temperature, heat generated by occurring electrochemical reactions and the heat dissipated from the fuel cell by active or passive cooling. (Fig.2) shows the block representation of the PEM FC thermal model as a MISO system with corresponding inputs and outputs. The generated fuel cell output current I_{FC} and voltage E_{cell} which are both results from electrochemical reactions, ambient temperature T_{amb} and initial temperature of the fuel cell stack are considered as inputs to the system. The only output of the system is the fuel cell stack actual temperature T_{FC} [8], [11].

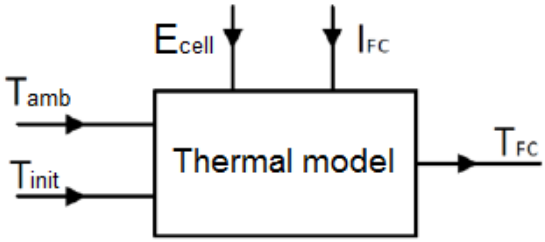

Fig.2. Block representation of PEM FC thermal model.

The transient change in fuel cell temperature can be represented by the following first order differential equation [8], [10], [11]:

$$\frac{dT_{FC}}{dt} = \frac{\Delta\dot{Q}}{M_{stack}c_{stack}}, \tag{5}$$

where $\Delta\dot{Q}$ represents a total heat flow inside the fuel cell stack [W], M_{stack} is a weight of the fuel cell stack [kg] and c_{stack} is an average heat capacity of the fuel cell stack [J/(K.kg)].

The total heat flow of the fuel cell stack can be calculated as a difference between generated and dissipated heat at any given time by equation [8]:

$$\Delta\dot{Q} = \dot{Q}_{gen} - \dot{Q}_{diss}, \tag{6}$$

where $\dot{Q}_{gen}$ is the generated heat flow [W] and $\dot{Q}_{diss}$ represents the heat dissipated from the fuel cell stack [W]. According to the forth mentioned equation, the value of the total heat flow will be positive when the temperature of the system is rising and negative when the temperature is decreasing. Its value can be also considered as a global heat gradient of the system.

The amount of generated heat flow $\dot{Q}_{gen}$ depends on the number of exothermic and endothermic electrochemical reactions occurring during the fuel cell operation as seen in [9], [10], [11].

The generated heat is causing an increase in fuel cell temperature, which in long enough time can reach values outside the operating temperature range of PEM FC. To maintain desired operating temperature of the stack, part of generated heat must be dissipated from the stack. Dissipation of heat from the considered air-cooled DEA PEM FC is caused by cooling system represented by cooling fan and by natural heat transfer mechanisms, namely convection and conduction heat transfer.

The equation of dissipated heat flow can be written as [10]:

$$\dot{Q}_{diss} = \dot{Q}_{fan} + \dot{Q}_{nat.conv}, \tag{7}$$

where $\dot{Q}_{fan}$ is a heat flow dissipated by the cooling fan [W] and $\dot{Q}_{nat.conv}$ is a heat flow dissipated from the surface of the FCs by natural convection [W]. The dissipation of heat by conduction heat transfer mechanism is not considered for the created model.

The following expression can be written for the heat flow dissipated by the cooling fan [8], [11]:

$$\dot{Q}_{fan} = \dot{m}_{air} c_{p,air} (T_{air,out} - T_{amb}), \tag{8}$$

where $\dot{m}_{air}$ is a mass flow rate of air [kg/s], $c_{p,air}$ is a specific heat capacity of the air [J/(K.kg)], $T_{air,out}$ is a temperature of the air exiting the cathode channels [°C]. The mass flow rate of air is generally dependent on stechiometry coefficient of the air and generated output power of the FCS.

Since there is no temperature regulation implemented in the model, the air mass flow rate $\dot{m}_{air}$ will be considered constant and its value is given by the amount of air flowing into system through the cooling fan [10], [11]. For the used PEM FC and other small fuel cells (FCs), it can be assumed that the temperature of exiting cathode air $T_{air,out}$ is equal to the actual fuel cell temperature T_{FC} [11].

Heat flow dissipated by means of the natural convection from the FCS surface is given by following relation [8], [11]:

$$\dot{Q}_{nat.conv} = \alpha_{conv} A_{stack} (T_S - T_{amb}), \tag{9}$$

where α_{conv} is a coefficient of convection [W/(K.m^2)], A_{stack} is the outer surface area of the FCs [m^2] and T_S represents the temperature of the surface area [°C], which is in considered model, equal to FCs actual temperature T_{FC}. For laminar flow of air, the convection coefficient for heat transfer from fuel cell stack surface to the ambient air reaches values from 5 to 10 W/(K.m^2) [11].

3 Complete Simulation Model

The complete simulation model of the thermal subsystem which was created utilizing the equations (5) - (9) can be seen in (Fig.3). Values of the required constants of the model are summarized in (Tab.1).

Table 1. Simulation parameters of the model.

Sign	Name	Value	Unit
M_{stack}	Weight of the FCs	0.25	[kg]
C_{stack}	Average heat capacity of FCs	50	[J/(K.kg)]
E_{Nernst}	Theoretical (Nernst) voltage of PEM FC	1.229	[V]
$\dot{m}_{air}$	Mass flow rate of air	4	[g/s]
$c_{p,air}$	Specific heat capacity of air	1004	[J/(K.kg)]
T_{amb}	Temperature of ambient air	25	[°C]
T_{init}	Initial temperature of FCs	25	[°C]
α_{conv}	Coefficient of natural convection	7	[W/(K.m^2)]
A_{stack}	Outer surface area of FCs	42	[cm^2]

In order to validate the performance of the created thermal simulation model, theoretical values were compared with the experimental data obtained from real fuel cell stack. The main part of the experimental work station was a commercial air – cooled PEM fuel cell stack HORIZON H – 12.

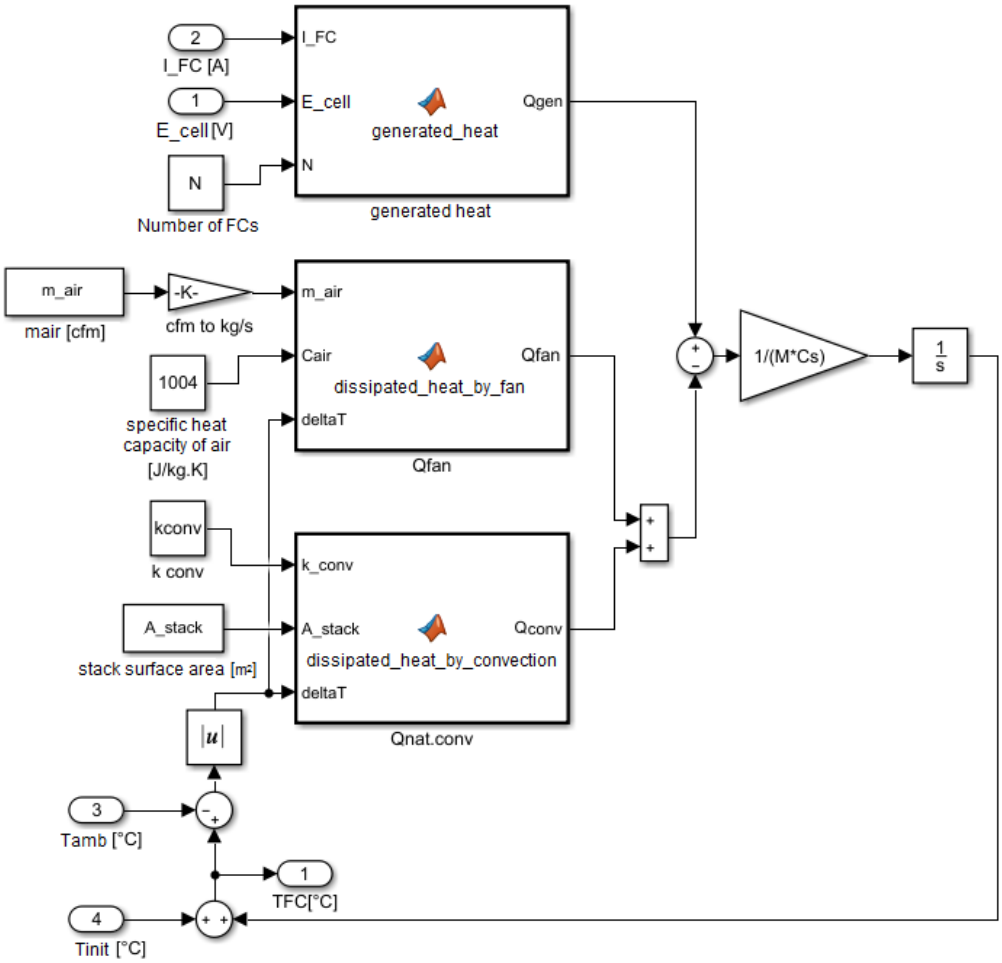

Fig.3. Simulation model – thermal subsystem.

4 Simulation Results and Discussion

With validated simulation model we proceeded to analyze the effects of temperature variations on fuel cell performance. The complex effect of temperature on FC losses can be seen on the polarization curves in (Fig.4). On the other hand, the higher temperature causes an increase in FC voltage in higher current densities. This is caused by the fact that the effect of lowering ohmic losses is more significant than the negligible increase in concentration losses. Since the peak power operating point also falls into the region of high current densities, increasing the temperature also rises the overall power output of the FCs which can be seen in (Fig.5).

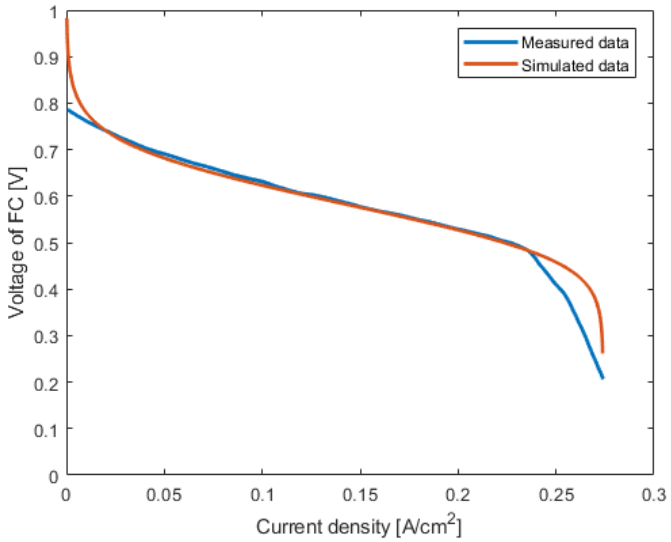

Fig.4. The effect of temperature on the character of polarization curve.

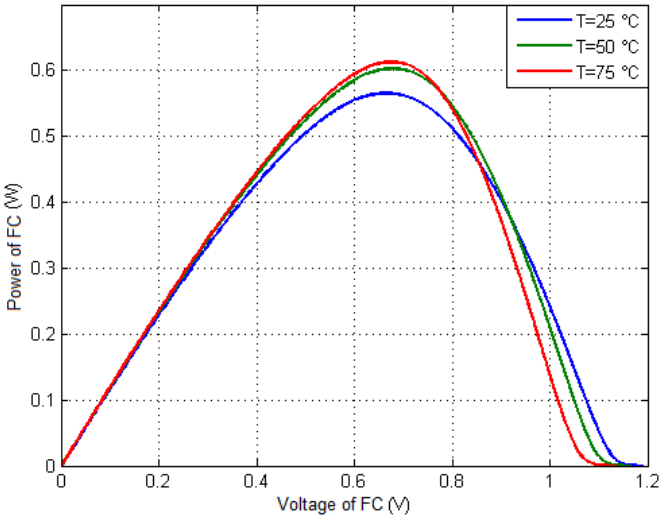

Fig.5. The effect of temperature on the value of one stack power.

The biggest change is achieved in the region of maximum peak power at voltages from 0.6 to 0.8V. Increase in the maximum power of the PEM FC is limited by the boiling point of water. Efficiency of the FC is also influenced by temperature.

On the contrary, in the region of high current densities, the efficiency of the stack increases. This is caused by shifting of the maximum power operating point towards higher values of current density and voltage.

In order to analyse dynamical properties of temperature and heat flow of the created thermal model, we carried out simulation of a transient response of FC the heat flow and temperature to the dynamic changes of generated electrical power.

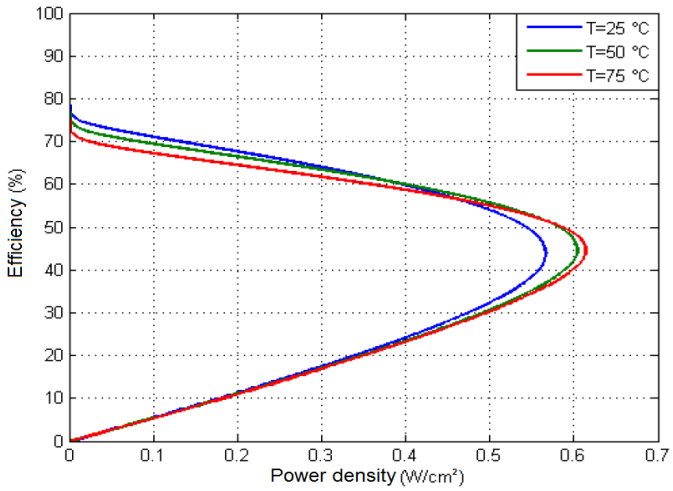

Fig.6. Efficiency of the FC as a function of power density.

Conclusion

For the purpose of analysing the effects of temperature on various parameters of PEM FCs in steady state and transient conditions without a need of experiments, an analytical zero-dimensional dynamic model was developed and validated to experimental data. The model is able to simulate electrochemical, thermodynamic and mass transport properties of the FCs. Regarding the scope of this paper, only thermal model was discussed in detail.

Efficiency of the stack exhibits a decrease in value at low current densities and increase at high current densities when the temperature rises. The maximum output power to temperature relation proved that the optimal temperature range for obtaining maximum power for the used PEM FCs is 60-80°C.

In our future work we will explore the influence of heat generation on water production and humidity inside the FCs which are highly interconnected effects.

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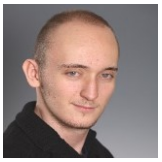
Authors



Ing. Matej Barát
Faculty of Mechanical Engineering,
Slovak University of Technology in Bratislava, Slovakia
Internal doctoral student, professional focus - hydrogen technologies
matej.barat@stuba.sk

Michal Stromko
Former fellow at Slovak University of Technology, Bratislava, Slovakia

prof. Ing. Viktor Ferencey, PhD.
Hydrogen Fuel Cells Slovakia, j.s.c. in Bratislava, Slovakia
Researcher in the field of hydrogen technologies
viktor.ferencey@gmail.com