Distributed high temperature PEM fuel cell modelling

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1. Introduction

High temperature PEM fuel cells (HT-PEMFC) suppose and advantage compared to their low temperature version [1], mainly because of their better higher CO tolerance, reaction kinetics and the lack of liquid water as a residual due to its operation temperatures between 120º and 180º, above water's boiling point [2]. Because of its ability to generate both electrical power and heat, HT-PEMFC are a good option for combined heat and power (CHP) applications [3] as long as a good way to convey heat through thermal management devices like heat exchangers.

In this article, an HT-PEMFC model based on partial differential equations of fluid dynamics and heat transfer, i.e. distributed model, is defined and introduced as well as the hypoteses assumed for its design. Its formulation, results and implications will be presented as well as its differences with other models presented in the literature [4].

2. Fuel cell model

2.1 HT-PEMFC description

The model defined is a 2-dimensional one with channels considered to be straight, i.e. without turns. There exist similar models in the literature for the case of low temperature PEMFC like [5] which have been analised and modified for the case of high temperature and its phenomenogical particularities, i.e. lack of liquid water, etc. The different fuel cell parts presented as well as the relationships imposed to variables between them are the ones shown in Figure 1, where $\dot{n}_{H_2}^A$, $\dot{n}_{H_2O}^A$, $\dot{n}_{O_2}^C$, $\dot{n}_{H_2O}^C$, $\dot{n}_{N_2}^C$ are the molar gas flows along the different layers of the fuel cell measured in mol/(l·s).

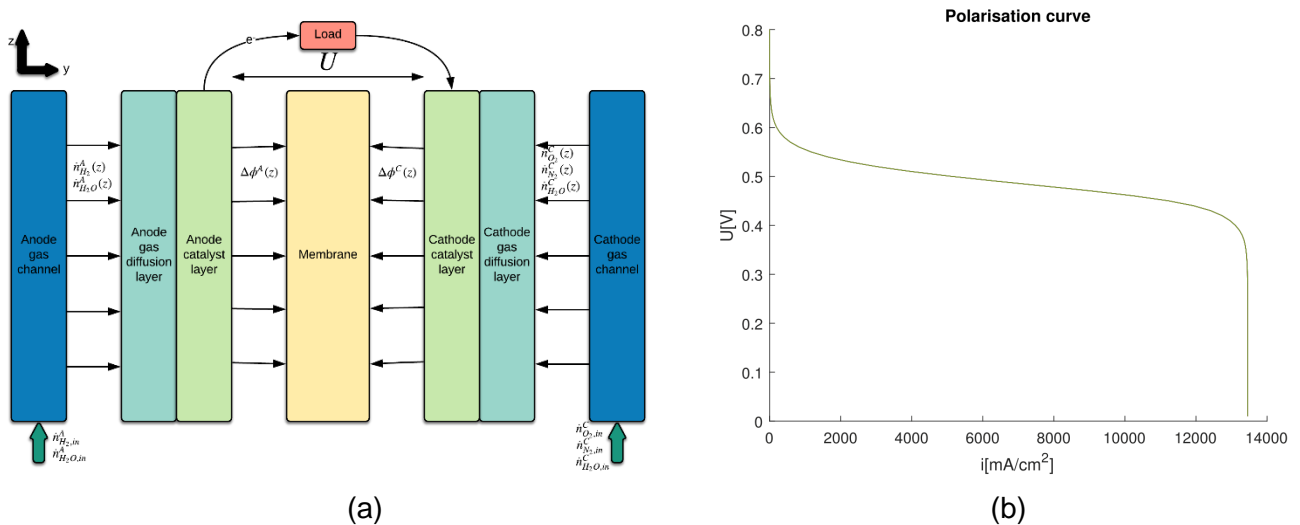(a)   (b)

Figure 1: (a) Model layers and relationship between variables. (b) Polarisation curve of the HT-PEMFC obtained from the model for a single cell.

The physical and chemical mechanisms and their correspondend equations considered in the modelling procedure are detailed as follows:

- Convective gas transport along anode and cathode gas channels.
- Darcy's law to link pressure drop and velocity within these gas channels.
- Energy transport due to convective flow, heat conduction according to Fourier's law, heat transfer between solid fuel cell parts and gas channels and enthalpy transport caused by mass flow from gas channels to the solid.
- Caloric equations of state, i.e. heat associated to a temperature increment as a function of specific heat of each substance.
- Stefan-Maxwell diffusion for ideal gases along gas diffusion layers.
- Species balances and chemical reactions on catalyst layers using Butler-Volmer kinetic rate expressions.
- Pseudo-homogeneous energy balance for the solid parts of the fuel cell.
- Species combination on the membrane.
- Charge balances at the anode and cathode double layers.

2.2 Model discretisation and linearisation

The resulting equations are nonlinear and include derivatives with respect to time and z spatial component (labelled in Figure 1a). Consequently, the defined model is discretised along z using finite differences to approximate its derivatives. After this, the model can be expressed as a function of state variables, i.e. those derived with respect to time. The form of the model is the following one (equation (1)):

$$\frac{d\boldsymbol{x}}{dt} = \boldsymbol{f}(\boldsymbol{x}, \boldsymbol{u}) \quad (1)$$

Where $\boldsymbol{f}$ is the vector function including all equations of the model, $\boldsymbol{x}$ is the state variables vector, i.e. variables including time derivative, $\boldsymbol{u}$ are the model inputs and t is the time. Variables composing $\boldsymbol{x}$ are:

- $c_{H_2}^A$ and $c_{H_2O}^A$ are anode hydrogen and water vapour concentrations in mol/l.
- $c_{O_2}^C$, $c_{N_2}^C$ and $c_{H_2O}^C$ are cathode hydrogen, nitrogen and water vapour concentrations in mol/l.
- T^A, T^C and T^S are temperatures for anode, cathode and solid parts respectively in K.
- $\Delta\varphi^A$ and $\Delta\varphi^C$ are anode and cathode proton potential difference measured in V.

If the time derivatives of $\boldsymbol{x}$ are set to zero a set of equilibrium points $(\boldsymbol{x}^*, \boldsymbol{u}^*)$ is found accordingly. It is important to note that, for the specific case of a fuel cell, plot of the set of its equilibrium points with voltage $U[V]$ and electrical current density $i[mA/cm^2]$ as the two variables selected for the axes is a characteristic result known as polarisation curve [1]. The polarisation curve obtained for the current model is the one on Figure 1b.

3. Results and Discussion

3.1 Electrical and thermal power

One of the main reasons to use HT-PEMFC is, as mentioned above, its ability to produce both electrical and thermal power. As seen in the previous section, the set of equilibrium points reachable by the fuel cell are plotted in Figure 1b, known as the polarisation curve. These equilibrium points can also be expressed as electrical and thermal power curves using the following expressions:

$$P_{electrical} = UI \quad (2)$$

$$P_{thermal} = P_{total} - P_{electrical} \quad (3)$$

These curves are plotted in Figure 2a in terms of the current $I[A]$. An important fact to know is that electrical current $I[A]$ and hydrogen flow $\dot{n}_{H_2}^A$ are related through a proportionality constant. It can be seen that both thermal and electrical power can be extracted to increase global system efficiency when using heat exchangers, batteries, tanks and other CHP system devices. It resembles concentrated parameters models in terms of shape and values [1]. The main challenge is designing a CHP system which takes the best profit of the thermal heat released.
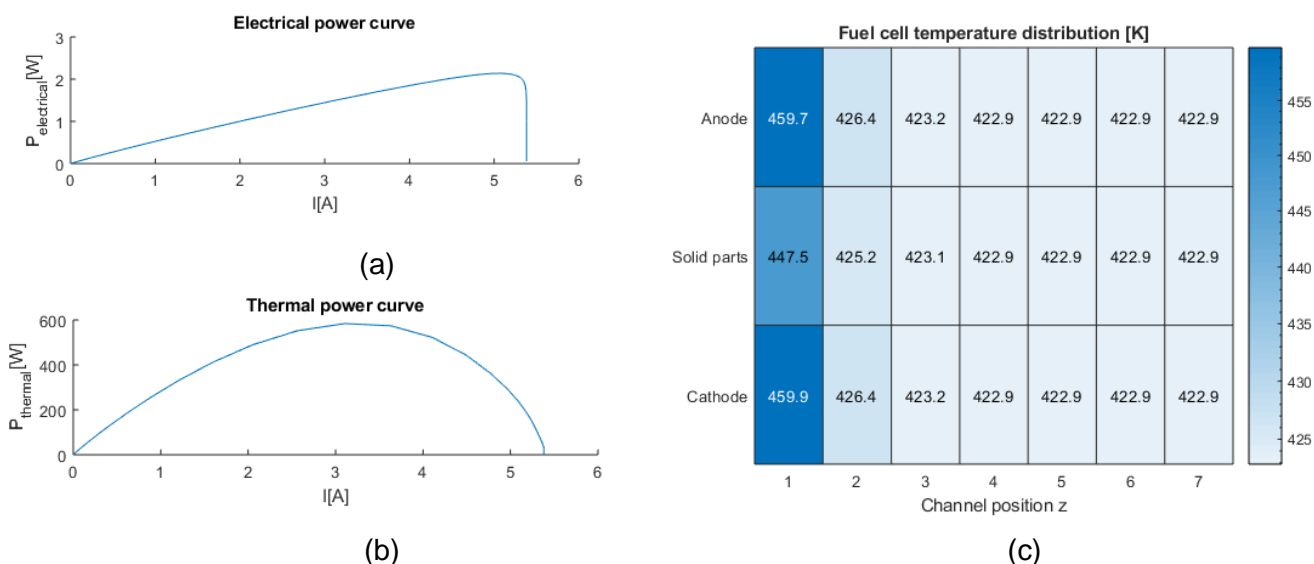
Figure 2: (a) Electrical power curve for the HT-PEMFC model. (b) Thermal power curve for the HT-PEMFC model. (c) Temperature distribution in Kelvin from anode to cathode (top to bottom).

3.2 Temperature distribution

The temperature distribution along the fuel cell varies from the inlet to the outlet of the gas channels (z coordinate) and along the fuel cell, i.e. from the anode to the cathode (y coordinate), as shown in Figure 2c. This distribution is the one to be seen in Figure 2c.

4. Conclusions

In this article, a distributed model based on partial differential equations for a HT-PEMFC is presented. The emphasys on CHP applications is briefly justified for the sake of the global system efficiency and process heat utilisation. This model has been spatially discretised and linearised so that it can be used for control purposes. The existence of a temperature gradient along the channel direction indicates that this kind of distributed model can be useful to optimize the heat transfer. As future work, model order reduction of the set of linearised models can be applied so that they become less computationally demanding as well. Additional experimental data not shown in this article are key to ensure that the model fits a specific real system.

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