

A Multiagent Model for PEM-Fuel Cell Microscopic Simulation

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Abstract—Since several years, multi-agent systems have been used for wide range of application areas and particularly in systems modelling and simulation. Those systems are based on the interaction of several individual components, called agents, which are proactive considering interaction with neighbours and with the surrounding environment. The IRTES-Set laboratory develops a PEM-Fuel Cell model for detailed layer level simulation based on multi-agent paradigm. Whatever the level of abstraction considered, modelling the electrochemical process requires at least: an electrochemical model, a fluidic model, and a thermal model. These elements are integrated into our simulation model at the microscopic level. The goal of this paper is to present a multi-physical micro-level PEM-Fuel Cell model by using a multi-agent approach.

I. INTRODUCTION

Multi-agent systems have become an appealing paradigm for problem solving [1], modeling and simulation of complex systems [2]. This paradigm provides a new approach to model such systems based upon the central notions of agents, their interactions and the environment they perceive and within they act. Multi-agent systems can be designed using two approaches. The first approach defines the system as a set of intelligent agents, each with individual cognitive abilities. The second approach introduces agents who do not possess individual cognitive abilities but are able to perform complex tasks through their interaction. Thus, intelligence is not in the individual components but emerges from multiple interaction between entities. This approach, called reactive, is particularly adapted to modelling and simulation of physical [3] or biological [4] based complex system. In this paper, we use the reactive approach to deal with the microscopic simulation of a PEM-Fuel Cell. Fuel

cell models using general structural approach (e.g. models clearly separated by geometry position and/or physical domains) have been published previously in the literature [12]-[16].

A 20-cell fuel cell stack model has been presented and validated experimentally in [12]. However no future information about model simulation performance has been given. A generalized fuel cell stack model including electrochemical, fluidic and thermal domain has been introduced in [13] by using a top-down approach and VHDL-AMS simulation language. Due to the VHDL-AMS limitation, the proposed model cannot perform multi-core simulation. A multi-core simulation model for fuel cell stacks electrochemical behaviour has been proposed in [14]. The model has been simulated in real time. However the multi-core approach has not been used in final simulation stage. A dynamic 5-cell stack model for solid oxide fuel cell [15] and a PEM-Fuel Cell model using differential-evolution-based method [16] have also been proposed recently for simulation and optimization purpose.

The fuel cell is a complex multi-physique device that involves electrochemical, fluidic and thermal phenomena. The complexity of physical equations for fuel cell modeling requires the use of advanced model simulation method, such as parallel simulation, for real time oriented fuel cell modelling applications (for example Hardware-in-the-Loop). The use of multi-agent approach for fuel cell modelling could improve the accessibility of the model components for parallel computation of fuel cell stack models. The paper is structured as follows. Section II exposes a state of the art on multi-agent simulation. Then section III describes the PEM-Fuel Cell governing equations for the multi-agent approach. Finally, after a presentation of several experimental results (section

IV), paper concludes by giving some future works.

II. MULTI-AGENT SYSTEMS AND SIMULATION

For a couple of years, a number of work have been dealing with multi-agent simulation. These works concern various domain such as Virtual urban simulation [5], pedestrian simulation [2], robotic and intelligent vehicle simulation [6]. Some of these are relies on multi-level modeling based on Computer-Aided Design (CAD) optimizations [7]. Mostly, multi-level simulation is composed of a fixed number of levels determined a priori by the designer of the model in relation with his experience. However, some multi-level simulations are based on dynamical level construction and on system's evolution. Multi-agent based approach deals generally with the study of emergent properties. The solution found is tied to specific case study based on mathematical inspiration [8], biological approach [9] or fully agent based considerations [10]. The approach proposed in this paper is based on a fixed hierarchical multi-agent model. Levels have been designed taking into account the general structure of a PEM-Fuel Cell used in a wide range of PEM research work. Each level corresponds to a specific point of view of the PEM-Fuel Cell function. For instance, stack level deals with the relation between cells at top level whereas Layer level deals with interaction between its components on electrical, fluidic and thermal views.

III. MODEL DESCRIPTION

A. Global overview: From stack to layer micro-model

On the top level, a PEM-Fuel Cell can be considered as a stack of several cells. The interactions between cells allows to obtain globally the expected function of fuel cell. Each cell, considered as an agent at stack level, is then composed of ten layers as shown in figure 1 in middle level. Each layer n is also considered as an agent interacting specifically with layers $n - 1$ and $n + 1$. Then, each layer agent is split into 3 agents: The Electrical Agent (EA), the Fluidic Agent (FA) and the Thermal Agent (TA). From the interactions between these three agents emerges the global behaviour of the layer. Figure 1 shows the agent structure of the PEM-Fuel Cell. Top level represents Cell agents in the stack. Middle level represents Layer agents in a cell. Then,

bottom level represents the electrochemical, fluidic and thermal aspects that characterise each layer.

The main interest of this structure is to be able to specify interaction between agents at each level of abstraction. However, in this paper, the focus is put on the microscopic level simulation (i.e. Layer Level), it is necessary to understand the role of each cell and of the layer before presenting each agent. Depending on its physical nature each agent does not necessarily includes the 3 physical aspects.

B. Layers micro-models

The goal of this section is to specify the behaviour of each micro-agent and the interactions between EA, TA and FA for each layer. Agents of Layer level can endorse one of the following roles: Electrochemical, Thermal and Fluidic. These three roles are specifically instantiated for each specific layer. Here is the detail of this instantiation. As already expressed, it should be noticed that these 3 agent models decomposition is not necessarily required for each layer. For instance, in the case of the cooling layer the electrochemical model is not needed.

1) *Cooling channel layer agents*: In this layer only the Thermal Agent is pertinent. The thermal dynamic response of a fuel cell depends on the thermal capacity of each layer in the cell. This dynamic can be generally described in a general form as:

$$(\rho \cdot V \cdot C_p) \cdot \frac{dT_{cv}}{dt} = \underbrace{\dot{Q}_{cond}}_{\text{conduction}} + \underbrace{\dot{Q}_{forced_conv}}_{\text{forced convection}} + \underbrace{\dot{Q}_{mass}}_{\substack{\text{convective} \\ \text{mass flow}}} + \underbrace{\dot{Q}_{sources}}_{\text{internal sources}} \quad (1)$$

where ρ is the mean layer volume density (kg/m^3), V is the layer volume (m^3), C_p is the layer thermal capacity ($J/(kg \cdot K)$) and stands for the different types of heat flows entering or leaving the layer volume (J/s): conduction, forced convection, convective mass flow and internal sources of heat. In the cooling channel layer, the forced convection phenomenon can be modelled by Newton cooling law:

$$\dot{Q}_{forced_conv} = h_{forced} \cdot S_{contact} \cdot (T_{fluid} - T_{solid}) \quad (2)$$

where h_{forced} is the forced convection heat transfer coefficient ($W/(m^2 \cdot K)$). The convective mass flow

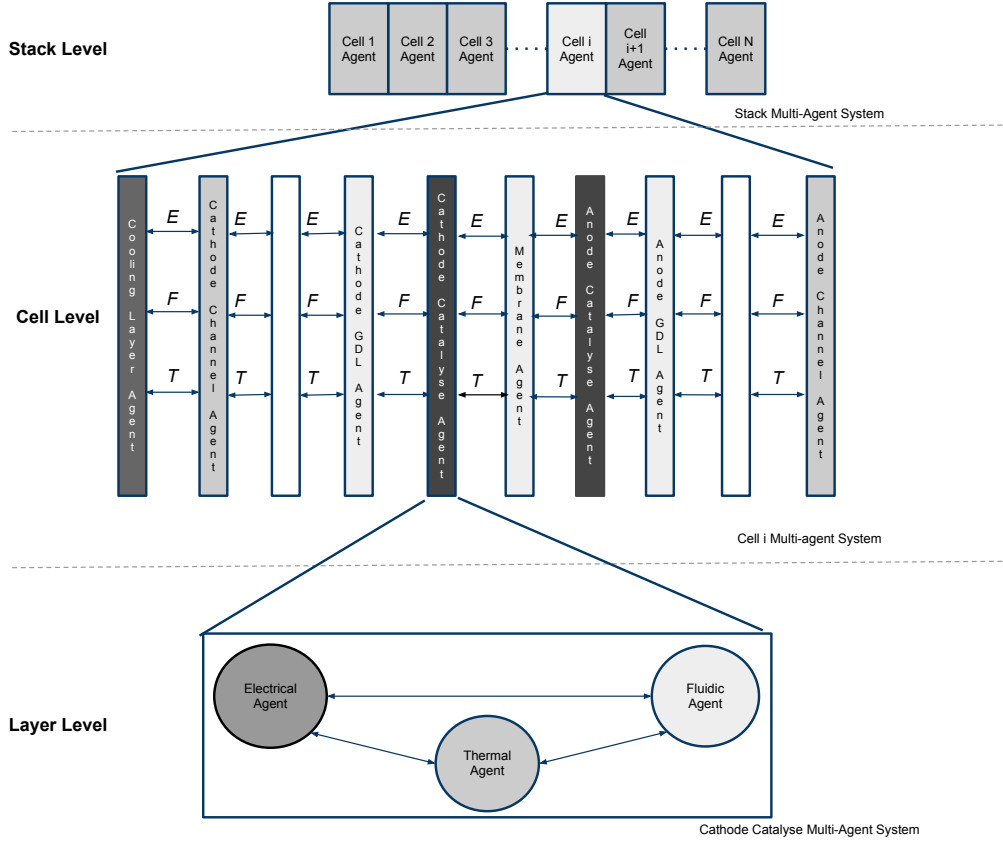


Fig. 1. Global architecture from stack to cell layers. (Blank rectangles correspond to cathode and anode gas supply channels)

due to the cooling fluid entering or leaving the fuel cell during operating could also be found in the cooling channel layer:

$$\dot{Q}_{mass} = \left[\sum_{fluid} (q_{fluid} \cdot C_{p,fluid}) \right] (T_{fluid} - T_{layer}) \quad (3)$$

Where q_{fluid} is the fluid mass flow rate (kg/s) entering or leaving the layer, C_p is the corresponding fluid thermal capacity ($J/(kg \cdot K)$).

2) Cathode/anode channel support layer agents:

As in cooling channel layer, only the Thermal Agent Behaviour is required. In the solid channel support layer, only the conduction phenomenon can be found in this layer. By applying the equation 4, the conduction heat transfer can be modelled by Fouriers Law:

$$\dot{Q}_{cond} = \frac{\lambda \cdot S_{contact}}{\delta} (T_{layer_1} - T_{layer_2}) \quad (4)$$

where λ is the material thermal conductivity ($W/(m \cdot K)$), S is the contact area (m^2) and δ the material thickness (m).

3) Cathode/anode gas supply channel layer agents:

• Fluidic Agent:

The fluid flows in the fuel cell gas supply channels are laminar flow. The gas pressure drop in the channels due to the mechanical losses can be expressed by the Darcy-Weisbach equation:

$$\Delta P = \frac{64}{Re} \cdot \frac{L}{2 D_{hydro}} V_S^2 \quad (5)$$

where D_{hydro} is the hydraulic diameter of the channels (m), V_S the mean fluid velocity in the channels (m/s), ρ_{ch} the channel gas density (kg/m^3), L the length of the channel (m) and Re , the fluid Reynolds number.

• Thermal Agent:

The thermal models for the cathode and anode gas supply channel are similar to the thermal model for the

cooling channels. The equations 1 to 3 are thus used. The coolant fluid parameters in those equations need to be replaced by those of air at cathode side and those of hydrogen at anode side.

4) Cathode/anode gas diffusion layer agents:

- Fluidic Agent:

The phenomenon of the multi-gas diffusion of each species (oxygen, hydrogen, nitrogen and water vapour) in the gas diffusion layers (GDL) can be described by the Stefan-Maxwell equation:

$$\Delta P_i = \frac{\delta_{GDL} R T}{P_{tot} S} \sum_{j \neq i} \frac{P_i \cdot \frac{q_j}{M_j} - P_j \cdot \frac{q_i}{M_i}}{D_{ij}} \quad (6)$$

where δ_{GDL} is the GDL thickness (m), S is the GDL layer section area (m^2), P_{tot} is the mean gas total pressure (Pa) in the GDL layer, M is the gas molar mass (kg/mol), j stands for species other than species i , and D_{ij} is the binary diffusion coefficient between the species i and j (m^2/s).

- Thermal Agent:

In the gas diffusion layer, the dominant thermal phenomenon is convective mass flow heat transfer which can be modelled by using equation 3 in equation 1. At cathode side, the diffusion gases are oxygen and vapour water. At anode side, the diffusion gases are hydrogen and vapour water.

5) Cathode/anode catalyst layer agents:

- Electrochemical Agent:

The cell reversible voltage can be obtained from the thermodynamic equation known as the Nernst equation:

$$E_{cell} = 1.229 - 0.85 \cdot 10^{-3} (T - 298.15) + \frac{R \cdot T}{2F} \ln \left(\sqrt{P_{O_2}} \cdot P_{H_2} \right) \quad (7)$$

where T is the temperature of the cell (K), P_{O_2} the oxygen pressure (atm) at the interface of cathode catalyst layer, P_{H_2} the hydrogen pressure (atm) at the interface of anode catalyst layer, R the ideal gas constant ($8.314 J/(mol \cdot K)$) and F the Faraday constant ($96485 C/mol$). The cell activation losses V_{act} (V) can be obtained from the Butler-Volmer equation:

$$i = i_0 \cdot S \left(e^{\frac{\alpha n F}{R T} V_{act}} - e^{-\frac{(1-\alpha) n F}{R T} V_{act}} \right) \quad (8)$$

where i is the stack current (A), S the catalyst layer section area (m^2), n the number of electrons involved in

the reaction, α the symmetry factor and i_0 the exchange current density (A/m^2).

- Fluidic Agent:

The gas mass flow rate (kg/s) through the gas diffusion layers to the catalyst layer is directly related to the stack current, as described in the following equations:

$$q_{O_2} = \frac{M_{O_2} i}{4F} \quad (9)$$

$$q_{H_2} = \frac{M_{H_2} i}{2F} \quad (10)$$

$$q_{H_2O, produced} = \frac{M_{H_2O} i}{2F} \quad (11)$$

- Thermal Agent:

The catalyst layers are where the electrochemical reaction takes place in a fuel cell. By applying equation 12, the main irreversible losses occur at the cathode catalyst layer due to entropy change in the reaction and the activation losses. These losses can be calculated as:

$$\dot{Q}_{source 1} = \underbrace{-i \cdot \frac{T \Delta S}{2F}}_{entropy \ change \ part} + \underbrace{i \cdot V_{act}}_{activation \ part} \quad (12)$$

Where ΔS is the entropy change ($J/(mol \cdot K)$) during the electrochemical reaction. In addition, the convective mass flow heat transfer in catalyst layers can be modeled by equation 3.

6) Membrane layer agents:

- Electrochemical Agent:

The cell resistive losses V_{ohm} are mainly due to the membrane resistance. These losses can be obtained by computing the membrane resistance and the Joules law:

$$V_{ohm} = R_{mem} \cdot i = \frac{i}{S} \int_0^{\delta_{mem}} r(T_{mem}) dz \quad (13)$$

where δ_{mem} is the membrane thickness (m) and $r(T_{mem})$ the membrane local resistivity ($\Omega \cdot m$). Thus, the cell overall voltage can be expressed as:

$$V_{Cell} = E_{Cell} - V_{act} - V_{ohm} \quad (14)$$

where E_{cell} is the single cell thermodynamic voltage (V), V_{act} the cell activation losses at catalyst layer (V) and V_{ohm} the cell resistive losses at membrane layer (V).

- Fluidic Agent:

The water balance in the membrane layer can be described by two different phenomenons: The electro-osmosis phenomenon in (15), and the back diffusion phenomenon in (16).

$$J_{drag} = \frac{n_{sat} \cdot \lambda(z)}{11} \cdot \frac{i}{2F} \cdot M_{H_2O} \quad (15)$$

$$J_{back_diff} = -\frac{\rho_{dry}}{M_n} \cdot D_\lambda \cdot \frac{d\lambda(z)}{dz} \cdot S \cdot M_{H_2O} \quad (16)$$

where $n_{sat} = 22$ is the electro-osmotic drag coefficient for maximum hydration condition, ρ_{dry} is the dry density of the membrane (kg/m^3), D_λ the mean water diffusion coefficient in the membrane (m^2/s), and M_n the equivalent mass of the membrane (kg/mol). The total water mass flow (kg/s) in membrane can be then expressed:

$$q_{H_2O,net} = J_{drag} + J_{back_diff} \quad (17)$$

This equation is a differential equation of $\lambda(z)$ derivated by z (the membrane diffusion-axis). By giving the boundary conditions for λ , the equation can be solved.

- Thermal Agent:

In the membrane layer, the convective mass flow heat transfer is due to the water flow in the membrane. The thermal model of the membrane layer is similar to the thermal model of gas diffusion layer by using equation 3. Besides, there is another heat source due to the Joule effect of the membrane resistance in this layer according to Joules Law:

$$\dot{Q}_{source2} = i^2 \cdot R_{mem} \quad (18)$$

The membrane layer thermal dynamic equation can thus be obtained by applying equation 1.

IV. MODEL EXPERIMENTAL VALIDATION

The proton exchange membrane fuel cell stack model presented in this paper has been validated experimentally in different physical domains with a 47 cell, air fed, 1 200 W Ballard Nexa fuel cell stack. The stack current profile that used for model validation has been shown in figure 2. The profile has incremental current steps at the beginning, followed by some rapid current variations in entire fuel cell stack current range.

The measured stack voltage response and the simulated stack voltage by model have been given in figure

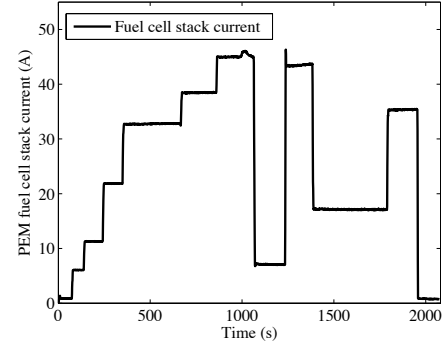


Fig. 2. Fuel cell stack current profile

3. The model predicted stack voltage has a very good agreement with the experimental data. The maximum voltage error for entire stack of 47 cells is less than 2 V. The stack voltage transient due to the stack thermal capacity have also been successfully predicted by the model. The voltage error at low stack current could be due to the empirical parameter values differences in Butler-Volmer equation for activation loss and in membrane resistance equation for ohmic loss.

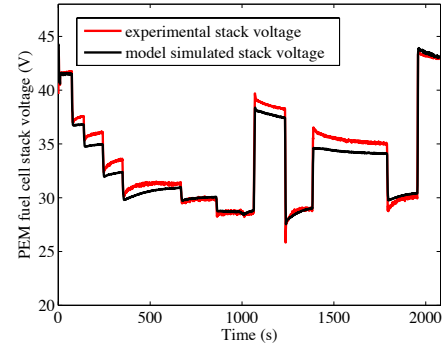


Fig. 3. Fuel cell stack current voltage (simulation and experimentation)

In thermal domain, the model predicted and the experimentally measured fuel cell stack temperature variations has been presented in figure 4. It can be concluded that, the model can predict the fuel cell stack temperature transient behaviour with a very high accuracy. The maximum stack temperature error between the model and real stack is less than 3.5 °C. In general, a fuel cell stack has a high thermal capacity due to its size. The thermal transient time can last up to some minutes. Thus, it is important to include the

stack thermal transient behaviour in the fuel cell model, if the stack operation condition varies in the time (for example, in transportation applications).

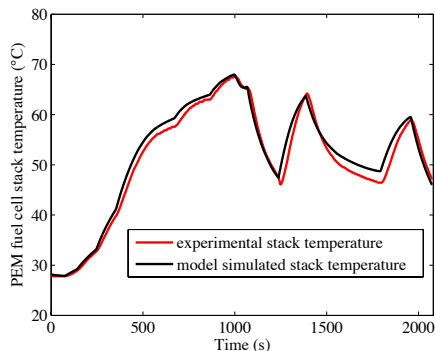


Fig. 4. Fuel cell stack temperature variation (simulation and experimentation)

V. CONCLUSION

In this paper, a microscopic simulation model for PEM-Fuel Cell stack has been presented. This model is based on multi-agent system paradigm and relies on the decomposition of each fuel cell layer into 3 agents (electrochemical, fluidic, thermal) which interact with each other and with their equivalent in adjacent layers. The combinations of these multiple interactions lead to a microscopic simulation of the fuel cell. Simulations and experimentations give some interesting results. We now plan to go further into this multi-agent modelling in order to obtain a multi-level fuel cell structure able to adapt to the implementation hardware.

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