# Species transport and water management in cathodic gas diffusion layer of PEM fuel cells

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#### Abstract

The proton exchange membrane fuel cell (PEMFC) is the largest used cell which is supplied whit hydrogen, but the correct water management is crucial for the optimum working. In order to analyse water behaviour within the cell, a transient mono-phase mathematical model is presented. The model accounts for gas mixture flow and species transport within the gas diffusion layer (GDL) in cathode side. This GDL is the layer which plays the main role in water evacuation in order to avoid pore blocking. The model concerns a given two-dimensional geometry where the governing differential equations are solved. The computational domain includes a gas diffusion layer, and a thin catalyst layer which is taken as an interface. The gas diffusion layer is a porous media which is characterised with a homogeneous morphological structure.

This numerical model is developed to simulate the transport operation in the cathode that is supplied with parallel (conventional) gas channel. The effective diffusivities according to the Bruggman correlation and Darcy's law for porous media are used instead of motion equation for the gas diffusion layer. In addition, the Fik equation is used to describe the oxygen reduction reaction (ORR) on the catalyst layer surface. The conservation equations for the gas diffusion layer are treated with finite volume method and solved numerically using an elaborate FORTRAN program.

The nature of the multidimensional transport in the cathode side of the cells is illustrated by the gas mixture velocity and species molar fractions. The obtained results are in qualitative agreement with recent experiments reported in the literature. A complement study performed with the model is presented and illustrates how fuel cell behaviour varies due to changes in parameters associated with the species transport and geometric structure.

Keywords: PEM fuel cells, Cathode, gas diffusion layer, water management.

# **1. INTRODUCTION**

A fuel cell is an electrochemical device that converts the chemical energy of a reaction directly into electricity as long we supply fuel. It is characterized by low chemical and acoustical pollution. In particular, PEM Fuel Cells is the most used in automotive application because it has a rapid starting. However, fuel cells need more researches in order to master operating aspects and costs. Among operating aspects we distinguish water management which get a great part of studies. In literature, we find complicate models for species transport, but the tendency is to formulate reduced and representative models. So, we represent a simple model which is specified in gas diffusion layer of cathode fig.1. This layer is the main element which regulates water management in fuel cells [1]. The model is inspired from Stockies et al. model [2] but with some simplifications: catalyst layer is supposed as interface [3], Burggman correlation is used to express diffusion coefficient and detailed boundary conditions given by BAO et al. are applied [4].



Figure 1. Gas diffusion layer structure

# 2. MATHÉMATICAL MODEL OF GAS DIFFUSION LAYER

#### 2.1. Hypothesis

- The cell temperature remains constant
- Gas diffusion layer is isotropic and homogeneous.
- All species are in the gaseous phase and the phase change of water was not included. The gas mixture is an ideal gas.
- Net water transport coefficient is constant along the x direction in an identical condition.
- Incompressible and laminar flow due to small pressure gradients and flow velocities.
- Gas mixture viscosity is constant; it is calculated from inlet conditions.
- Motion equations are reduced to Darcy law.
- Calculus domain is bidimensionnel.

#### 2.2. Governing equations

$$\frac{\partial \rho}{\partial t} + \nabla .(\rho \mathbf{U}) = 0 \tag{1}$$

$$\mathbf{U} = -\frac{K}{\varepsilon \mu} \nabla P \tag{2}$$

$$\frac{\partial C_k}{\partial t} + \nabla \cdot (\mathbf{U}C_k) = \nabla \cdot (D_k^{eff} \nabla C_k)$$
(3)

Mixture velocity **U** is expressed with ideal gas law: P = CRT

Mixture concentration *C* is a function of mixture density  $\rho$ , Oxygen concentration *C*<sub>0</sub>, water vapour concentration *C*<sub>V</sub> and species molar mass (*M*<sub>0</sub> : *Oxygen*, *M*<sub>V</sub> : *water vapour*, *M*<sub>Z</sub> : *Nitrogen*) :

$$C = \left[\rho + (M_{z} - M_{o})C_{o} + (M_{z} - M_{v})C_{v}\right] / M_{z}$$

Effective diffusion coefficients  $D_k^{eff}$  are obtained with Bruggman correlation also it depend on temperature and pressure [5]:

$$D_k^{eff} = \varepsilon^{1.5} D_k = \varepsilon^{1.5} D_{k0} (T/353)^{1.5} (1/P)$$

*K*,  $\mu$ ,  $\varepsilon$ ,  $D_{k0}$  are respectively: permeability, viscosity, media porosity and specie diffusion coefficients at standard conditions

#### 2.3. Boundary conditions

The unknowns are  $\rho$ ,  $C_{O2}$ ,  $C_{H2O}$ . As in fig.2, at the extern domain boundaries we use no-flow conditions except at air inlet and catalyst layer.

2.3.1. y=0,  $0 \le x \le W/2$  at air entry, it is assumed by average values in the gas chanel :



Figure 2. Calculs domain

Average values are calculated between inlet and outlet gas channel, outlet species molar fractions  $X_{\rho}^{out}$ ,  $X_{V}^{out}$  depend on inlet fractions  $X_{\rho}^{in}$ ,  $X_{V}^{in}$  and stoichiometric ratio  $\xi$  [4]:

$$X_{V}^{out} = \frac{\xi \cdot X_{V}^{in} + 0.42(1+2\alpha)(1-X_{V}^{in})}{\xi + 0.21(1+2\alpha)(1-X_{V}^{in})} \qquad X_{O}^{out} = \frac{0.21(\xi-1)(1-X_{V}^{in})}{\xi + 0.21(1+2\alpha)(1-X_{V}^{in})}$$

 $\alpha$  : net water transport coefficient in membrane

2.3.2. y=0,  $W/2 < x \le W$  on current collector plate, it is impermeable boundary (wall), so flux and velocities are nul :

$$\partial C_k / \partial y = 0$$
,  $\mathbf{U} = 0$ 

- 2.3.3. x=0 et x=W at symetry axes which passed in opning channel midle, so symetry conditions are appiled.
- 2.3.4. y=H at catalyst layer, where electrochimecal reaction is assumed instantanous, diffusive flux  $J_k$  depend on current density I which depend on distance x as shown in fig..3, curve traced by BAO et al.[4], is interpolated in polynomnal expression.



Figure 3. Current density curve

#### **3. NUMERICAL PROCEDURES**

Finite volumes method [6] with central difference interpolation is used in spatial discritisation of governing equations. Implicit time discretisation is applied for the temporal variable. Linear equation system is resolved with Gauss-Seidel algorithm. Calculation is performed with an elaborate FORTRAN program by using base case parameters given in table 1.

Symbol	Designation	value
Н	Gas diffusion layer thickness cm	0,03
W	Gas diffusion layer width cm	0,115
Ι	Average current density A/cm <sup>2</sup>	1,0
Р	Fuel cells pressure $g/cm.s^2$	$0,3\ 10^6$
3	Gas diffusion layer porosity	0,5
R	Universal gas constant $m^2/mol s^2 \circ K$	8.3145 10 <sup>7</sup>
Т	Fuel cells temperature K°	343
$\mu_O$	Oxygen Viscosity (at T=343°K) g/cm.s	32,30 10 <sup>-5</sup>
$\mu_V$	Water vapour viscosity (à T=343°K) g/cm.s	$11,72 \ 10^{-5}$
$\mu_Z$	Nitrogen viscosity (à T=343°K) g/cm.s	20,03 10 <sup>-5</sup>

K	Gas diffusion layer permeability cm <sup>2</sup>	10 <sup>-8</sup>
F	Faraday constant C/mol	96487
α	Net water transport coefficient	0,064
$X_{O}^{in}$	Oxygen molar fraction at gas Channel inlet	0,19
$X_V^{in}$	Water vapour molar fraction at gas Channel inlet	0,066
ξ	Stoichiometric ratio	2.5
$D_{\theta V}$	STD water vapour diffusion coefficient cm <sup>2</sup> / s	0,389
$D_{\theta 0}$	STD Oxygen diffusion coefficient cm <sup>2</sup> /s	0,324
$\delta P$	Pressure difference between inlet and outlet of gas channel g/cm.s <sup>2</sup>	2

# 4. RESULTS AND DISCUSSIONS

#### 4.1 Oxygen concentration profile

Curves shown on fig.4 represent oxygen molar fraction in GDL, it is in good concordance with experimental results of BAO et al. [4]. Oxygen concentration decrease in the positive sense of y axe as well as oxygen is consumed. Current collector plate narrow air entry so oxygen transport slows down in positive sense of x axe from entrance until collector plate middle. Minimum concentration set on catalyst surface at collector plate middle axe.

# 4.2 Water vapor concentration profile

Curves shown on fig. 5 represent water vapour molar fraction in GDL, it is in good concordance avec with experimental results of BAO et al. [4]. Water vapour concentration increases in the positive sense of y axe as well as water vapour is produced and reach its maximum at catalyst surface on collector plate middle axe. Water is assumed that exist only in vapor state. However hypothesis, if chemical reaction rate is great water condensation took place. In This case appear a biphasic flow. But according to Wang et al. analysis, monophasic flow is a good approximation for testing fuel cells performance in moderate current densities interval (about  $0.6 \text{ A/cm}^2$ ). For high current, excess of liquid water in GDL can embarrass Oxygen transport to reach catalyst sites, so for remedying this inconvenient it need to make light correction on porosity in order to coincide simulation with experimental results. However, recent biphasic models indicate that is only 5% of liquid water effect when operating at  $1.5 \text{ A/cm}^2$ , so liquid water influence is too little.





Figure 5. Water vapour molar fraction

#### 4.3 Mixture velocity Profile

Velocity profile shown on fig. 6 is in good concordance with Mingruo et al. [7] results. At GDL entry, Mixture velocity has vertical direction, then it incline gradually to horizontal positive sense because it encounter membrane obstruction which is impermeable against transported species. Horizontal component became null on median axe of collector plate, because it encounter opposite flux which comes from adjacent channel.



Figure 6. Mixture velocity profil (for half cell)

#### 4.4 Effet of parameter variations

In fact, GDL partial model does not permit testing effect on fuel cells power, but it allows showing influence on water management. For present system with conventional gas channel, we take as indicator a point from more critical field which located on median axe of collector plate at catalyst neighbours. So we choose this point for controlling water vapour concentration.

## 4.4.1 Effect of Air humidification

As shown on fig. 7, the decrease in air humidification leads to decreasing water vapor concentration in GDL, so with little air humidification leads to fuel cells drying.

#### 4.4.2 Effect of pressure

Net water transport coefficient is assumed as constant so we take identical pressure in anode and cathode. As shown in fig. 8 water vapor concentration increase with increasing pressure.



Figure 7. Effect of air humidification

Figure 8. Effect of pressure

# 4.4.3 Effet of air stoichiometric ratio

Fig. 9 shows the effects of air stoichiometric ratio on water vapour transport. Water vapor concentration in GDL decreases with increasing air stoichiometric ratio. But, we know that flow air is supplied by air compressor and more flow need more energy, so this parameter should be optimised. Concentration in GDL decreases with increasing air stoichiometric ratio. But, we know that flow air is supplied by air compressor and more flow need more energy, so this parameter should be should be optimized.

# 4.4.4 Effet of gas diffusion layer thickness

In base case, 0,03 cm of GDL thickness is one of the smallest values used in PEM fuel cells. As shown on fig. 10, Water vapour concentration in GDL increases with increasing GDL thickness. This increase is due to a long distance crossed by water evaporation to reach gas channel.

# 4.4.5 Effet of collector plate width

For this manipulation, gas channel width and cell width are fixed, we change collector plate width. As shown on fig. 11, Water vapor concentration in GDL decreases with decreasing collector plate width. This decrease is due to the reduction of obstacle surface which embraces

exhaust air. But we note that any reduction of collector width increase electric resistance so this dimension should be optimized.



Fig. 9 Effect of air stoichiometric ratio Fig. 10 Effect of GDL thickness Fig. 11 Effect of collector plate with

## 5. CONCLUSION

The bidimensionnel model present a good approximation tridimensionnel flow in gas diffusion layer, but water monophasic state (vapour) need light porosity correction in order to make better simulation for high water production. Although, recent biphasic researches play down its effect, water management in GDL needs more analysis in order to clarify biphasic flow in high current interval. This effect is evaluated about 5% at current density more than 1,5  $A/cm^2$ .

Widely, Water vapour concentration decrease with increasing air stoichiometric ratio (from 2,5 to 4,5). But, high air flow needs more energy which is consumed by air compressor, so there is an optimal flow which presents the maximum system efficiency. Water vapour concentration decreases with increasing collector plate width from 0,0575 cm to 0,0143. But, we should take account that any collector surface reduction causes electrical resistance increase, so this dimension must be optimised.

In order to draw cell polarisation curve which used to compare simulation with experimental results, a cell complete model is scheduled for the future work.

# References

- 1. James Larminie, Andrew Dicks, "Fuel Cell Systems Explained", Second Edition, John Wiley & Sons Ltd, England, 2003.
- 2. K. Promislow and J. M. Stockie. "A finite volume method for multicomponent gas transport in a porous fuel cell electrode". *Int. J. Numer. Meth. Fluids* 2001; 00:1–35
- 3. J.J. Hwang, C.K. Chen, R.F. Savinell, C.C. Liu et J. Wainrigth, (2004), "A three-dimensional numerical simulation of the transport phenomena in the cathodic side of a PEMFC", Journal of Applied Electrochemistry 34: 217–224, 2004. 217, 2004.
- 4. Bao C., Ouang M. et Yi B.(2006) "Analysis of Water Management in Proton Exchange Membrane Fuel Cells", J. Tsinghua Science and Technologie ISSN 1007-0214 10/21 pp54-64
- 5. S. Um, C.Y. Wang, K.S Chen, "Computational Fluid Dynamics Modeling of Proton Exchange Membrane Fuel Cells," J. Electrochem. Soc., Vol 147, No. 12, 2000,pp.4485-4493,.
- 6. Suhas Patankar, "Numerical Heat Transfer and Fluid Flow," Hemisphere, Washington D.C., 1980.
- 7. Mingruo Hu, Xinjian Zhu, Minghua Wang, Anzhong Gu, Lijun Yu, "Three dimensional, two phase flow mathematical model for PEM fuel cell": Part II. Analysis and discussion of the internal transport mechanisms, J. Energy Conversion and Management 45 (2004) 1883–1916.