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Modeling of Crossover Phenomenon in Liquid Feed Direct Methanol Fuel Cells

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Abstract: Increasing energy consumption and global warming problem make use of renewal energies inevitable. Among these energy resources, fuel cells are interesting due to almost inexpensive raw materials and high performance. In recent years, the Direct Methanol Fuel Cells (DMFC) have been increasingly interesting because of its low temperature over the other fuel cells, removing problems due to storage and conversion of hydrogen, ease of operating and simplicity for transportation applications. In the first section of this study, 3-D modeling of DMFC is solved by use of the finite element method. The obtained results show good agreement with experimental data which are reported in their paper. In this study, a two dimensional, isothermal, steady-state model is developed for DMFC. The model is accounting for mass balances, the charge balances, electrochemical reactions and the mass transport phenomena. Diffusion and convective effects as well as crossover of methanol are considered in this model. The governing equations are solved using COMSOL software. The results are reported as methanol concentration profile and methanol flux in gas diffusion, catalyst and membrane layers; oxygen concentration profile in cathodic catalyst layer; anodic and cathodic overpotentials changes through catalyst layer, and finally, the cell voltage versus different current densities. The results show that methanol concentration reduces through the layers and reaches zero in the interface of the membrane and catalyst layer. At lower methanol concentrations, the profiles have the same concentration gradient and increase through the layers as current density increases. Furthermore, anodic and cathodic overpotentials increase as current density increases. Oxygen concentration decreases through catalyst cathodic layers.

Keywords: DMFC, Fuel Cell Modeling, Methanol Crossover

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1. Introduction

Fuel cell is a device used to convert chemical energy to electricity. It is mainly comprised of cathode electrode, anode electrode and electrolyte. Direct Methanol Fuel Cell (DMFC) is a sub-type of polymer electrolyte membrane fuel cells in which methanol is oxidized in anode and oxygen is reduced in cathode. Due to its high energy density, safe fuel storage and transportation, relatively simple structure, and low environmental pollution [1] DMFCs are considered to be the best alternative to conventional battery systems in portable electronic devices (e.g., laptops, cell phones) and also as a possible future alternative for vehicles and transportation [2].

In the field of DMFC design and operability, one of the most important challenges is methanol crossover through the polymer electrolyte membrane. Crossover is driven mostly by of diffusion, electro-osmosis and transfer due to pressure gradient. These contributors manifest differently under different operational conditions. In higher temperatures and methanol concentrations permeation is dominant and since pressure is the same on both sides of anode and cathode, crossover has more impact in the cathode layer. The methanol crossover not only is responsible for the loss of more than 30% of fuel but also results in mix potential in cathode and toxicity of the cathode catalyst layer (CCL). The CO_2 released in the reaction results in toxicity of CCL which decreases the efficiency of the fuel cell. Both Crossover and toxicity effects are included in the present simulation.

Sundmacher et al. [3] have studied the dynamics of a DMFC. They analyzed the voltage of a cell with dynamic methanol injection and developed a model that includes mass balance in anode, charge balance in both electrodes and rate of electrochemical reactions. Experimental results show that dynamic methanol injection, decreases methanol transmitting through membrane and consequently cathode's potential increases. Also mass transfer coefficient increases with feed methanol concentration. Whereas in their model it only depends on feed flowrate, although it still shows the importance of other phenomena like mass transfer on anode's surface.

Ge et al. [4] conducted an experimental study on direct methanol fuel cells. Their experiment shows that humidification of cathode does not have much effect on the cells efficiency. Also the structure of cathode and operational conditions have an important role in DMFC design. As a rule of thumb, cell efficiency improves with air flowrate intensity but it's less effective than anode flowrate and it becomes almost ineffective after a specific value.

A theoretical model of the collective electrode-membrane of a DMFC including methanol and water crossover has been developed by Yin et al. [5]. The model was limited to electrode-membrane and excludes flow channels. Because of high methanol concentration in cathode it was assumed that crossovered methanol is completely consumed in the interface of cathode diffusion layer and membrane and carbon dioxide bubbles produced in anode are negligible. Then water mass conservation was applied to Anode Diffusion Layer (ADL) where water flowrate is substituted with Darcy's law. Water flowrate in the membrane and methanol flowrate in ADL were defined by means of electro-osmotic

drag, pressure gradient, permeation and convection respectively.

By studying of the aforementioned models it can be deduced that the proposed models either focus on one or a few specific layers and the corresponding effective parameters. In most fuel cell models steady and isothermal conditions is assumed and pressure drop in layers is neglected. Since experiments are case specific and cannot be used for designing a new fuel cell and numerical methods are slow and not suited to fuel cell behavior prediction, therefore we have used a 3-D model for simulation and analysis in COMSOL software which is both fast and accurate.

2. Governing equations

The phenomena that occurs due to the combination of physics and chemistry in fuel cells are very complex and sometimes unknown so its models are not necessarily accurate and need to be validated by experimental results. In this model, it is assumed that flow in channels is uniform, electron and proton conductivity of the layers are constant and there is no total pressure drop in electrode layers. The main assumptions in the mathematical formulations are: (i) the flow in channels is single phase, (ii) the membrane is fully hydrated, (iii) isothermal condition, (iv) steady-state operation, (v) the electrolyte is solid and an insulator.

Charge conservation

According to Ohm's law current density for electron and proton can be expressed as (l and s indexes describe the liquid electrolyte and electrode)

$$i_l = -\sigma_l \nabla \phi_l \qquad \text{(ACL, M, CCL)} \qquad (1)$$

$$i_s = -\sigma_s \nabla \phi_s \qquad \text{(ABL, ACL, CCL, CBL)} \qquad (2)$$

Also according to electrolyte neutrality no electric charge is consumed or produced in backing layers or the membrane

$$\nabla . i_s = 0 \qquad \text{(ABL, CBL)} \qquad (3)$$

$$\nabla . i_l = 0 \qquad \text{(M)} \qquad (4)$$

Since electrons and protons move in opposite directions, in ACL and CCL we have

$$\nabla . i_l = -j_a \qquad \text{(ACL)} \qquad (5)$$

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$$\nabla . i_s = j_a \qquad \text{(ACL)} \tag{6}$$

where j_a and j_c are volumetric current densities in anode [6] and cathode respectively and given as

$$j_a = A_v j_{oa}^{\text{ref}} \left(\frac{C_M}{C_{\text{MeOH}}^{\text{ref}}} \right)^{0.5} \exp\left(\frac{\alpha_a F \eta_a}{RT} \right) \tag{7}$$

In the equation η_a the overpotential is expressed as

$$\eta_a = \phi_s - \phi_l - E_a^{\text{Eq}} \tag{8}$$

Cathode catalyst layer charge conservation can be expressed using these equations

$$\nabla . i_l = -j_c \qquad \text{(CCL)} \tag{9}$$

$$\nabla . i_s = j_c \qquad \text{(CCL)} \tag{10}$$

$$j_c + j_{\text{xover}} = A_v j_{oc}^{\text{ref}} \left(\frac{C_{O_2}}{C_{O_2}^{\text{ref}}} \right) \exp\left(\frac{-\alpha_c F \eta_c}{RT} \right) \tag{11}$$

Here j_{xover} represents methanol crossover volumetric current density

$$j_{\text{xover}} = \frac{6 F \dot{N}_{\text{MeOH}}^{\text{M/CCL}}}{t_{\text{ccl}}} = 6 n_d^{\text{MeOH}} j_a \qquad j_c = j_a \tag{12}$$

$$\eta_c = \phi_s - \phi_l - E_c^{Eq} \tag{13}$$

By combining equations (11) and (12) we get

$$j_c = \frac{A_v j_{oc}^{\text{ref}} \left(\frac{C_{O_2}}{C_{O_2}^{\text{ref}}} \right) \exp\left(\frac{-\alpha_c F \eta_c}{RT} \right)}{1 + 6 n_d^{\text{MeOH}} j_a} \tag{14}$$

Momentum conservation and continuity

Continuity in steady state for fuel and air channels and backing layers can be written as

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$$\rho \nabla . u = 0 \tag{15}$$

and for catalyst layers as

$$\rho \nabla . u = \sum S_{u,k} M_k \tag{16}$$

Momentum conservation can be expressed generally with [6]

$$\frac{\rho}{\varepsilon^2}(u.\nabla)u = -\nabla P + \nabla r + S_u \tag{17}$$

where S_u can be taken as zero for both channels and be obtained from Darcy-Weisbach law for other layers

$$S_u = 0 \tag{18}$$

$$S_u = -\frac{\mu}{K}u \tag{19}$$

Inlet mean velocities are [6]

$$v_{fc,in} = \frac{\zeta_a i_{ref} l_{cell} w_{cell}}{6 F C_{MeOH}^{fc,in} t_{fc} w_{fc}} \tag{20}$$

$$v_{ac,in} = \frac{\zeta_c i_{ref} l_{cell} w_{cell}}{4 F C_{O_2}^{ac,in} t_{ac} w_{ac}} \tag{21}$$

Species transport

Methanol

Methanol enters the cell through the fuel channel, most of it enters the ACL and the remainder exits the cell through the channel. Since we have no electrochemical reaction methanol flux is constant in this layer. Methanol molar flowrate and its transport equations can be written as

$$\dot{N}'' = -D\nabla C + uC \tag{22}$$

$$\nabla . N'' = C \tag{23}$$

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$$\nabla.(-D\nabla C) + u.\nabla C = 0 \tag{24}$$

In anode backing layer porosity needs to be taken into account too, so we have

$$\dot{N}'' = -D_{eff}\nabla C + uC \tag{25}$$

$$\nabla.(-D_{eff}\nabla C) + u.\nabla C = 0 \tag{26}$$

$$-D_{MeOH}^{eff,ABL}\frac{d^2 c_{MeOH}^{ABL}}{dx^2} + \frac{M_{H_2O}N_{H_2O}^{ABL}}{\rho_{H_2O}}\frac{dc_{MeOH}^{ABL}}{dx} = 0 \tag{27}$$

Effective diffusivity in porous media obtained from [7]

$$D_{eff} = \varepsilon^{1.5}D \tag{28}$$

where ε is porosity and D is species diffusion coefficient. Because of reactions in the cathode catalyst layer, methanol transfer is the sum of diffusion in porous media and transport effects. Production of proton results in gravitation of methanol to the membrane so we have to consider electro-osmotic effects too. Hence methanol flux and transport equations are expressed as

$$\nabla\dot{N}'' = \frac{-6}{nF} \qquad n = 6 \tag{29}$$

$$\dot{N}'' = -D_{eff}\nabla C + uC + n_d^{MeOH}\frac{i_i}{F} \tag{30}$$

By combining eq. (30) with eq. (29) and (6) we will have the following equation

$$\nabla.(-D_{eff}\nabla C) + u\nabla.C = \frac{-j_a}{F}(1 + n_d^{MeOH}) \tag{31}$$

In fuel channel and the backing layer, drag coefficient of methanol solution is assumed to be constant but in the ACL we have [7]

$$-D_{MeOH}^{eff,ACL}\frac{d^2 C_{MeOH}^{ACL}}{dx^2} + \frac{M_{H_2O}N_{H_2O}^{ACL}}{\rho_{H_2O}}\frac{dC_{MeOH}^{ACL}}{dx} - \frac{-j_a}{F}(1 + n_d^{MeOH}) = 0 \tag{32}$$

$$n_d^{MeOH} \cong n_d^{H_2O}\frac{C_{MeOH}}{C_{H_2O}} \tag{33}$$

There is no electrochemical reaction in the membrane and it is porous too so the equations become

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similar to that of the ABL and in differential terms we have

$$-D_{MeOH}^{eff,M}\frac{d^2C_{MeOH}^M}{dx^2}+\frac{M_{H_2O}N_{H_2O}^M}{\rho_{H_2O}}\frac{dC_{MeOH}^M}{dx}=0 \tag{34}$$

In CCL crossovered methanol's reaction in interface of membrane and catalyst layer happens instantly and all of it is consumed. So we only need to consider oxygen mass balance which will be explained in its corresponding section.

Water

Water transfer equations in fuel channel and ABL is similar to equations (22) to (28). For water transport in ACL we have [6]

$$\dot{N}''=-D_{eff}\nabla C+uC+n_d^{H_2O}\frac{i_l}{F} \tag{35}$$

$$\nabla.(-D_{eff}\nabla C)+u\nabla.C+\frac{n_d^{H_2O}\nabla.i_l}{F}=\frac{-j_a}{6F} \tag{36}$$

Combining the above equation with eq. (6)

$$\nabla.(-D_{eff}\nabla C)+u\nabla.C=\frac{-j_a}{F}\left(\frac{1}{6}+n_d^{H_2O}\right) \tag{37}$$

$$-D_{H_2O}^{eff,ACL}\frac{d^2C_{H_2O}^{ACL}}{dx^2}+\frac{M_{H_2O}N_{H_2O}^{ACL}}{\rho_{H_2O}}\frac{dC_{H_2O}^{ACL}}{dx}-\frac{-j_a}{F}(\frac{1}{6}+n_d^{H_2O})=0 \tag{38}$$

Oxygen

Oxygen equations are similar to methanol's except in CCl where we have a sink term in the transfer equation due to electrochemical reactions. Molar flowrate of oxygen in CCl can be expressed as [7]

$$\dot{N}''=-D_{eff}\nabla C+uC \tag{39}$$

Contributors to oxygen mass flux are oxygen reduction in this layer and crossovered methanol so we have

$$\nabla\dot{N}''=-1.5\frac{j_c+j_{xover}}{nF}\qquad n=6 \tag{40}$$

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$$j_{\text{xover}} = 6n_d^{\text{MeOH}} j_a \qquad\qquad j_a = j_c \tag{41}$$

$$\nabla.(-D_{\text{eff}}\nabla C) + u\nabla.C = \frac{-1.5}{6F}j_c\left(1 + 6n_d^{\text{MeOH}}\right) \tag{42}$$

$$-D_{O_2}^{\text{eff,CCL}}\frac{d^2 C_{O_2}^{\text{CCL}}}{dx^2} + \frac{M_{O_2} N_{O_2}^{\text{CCL}}}{\rho_{O_2}}\frac{dC_{O_2}^{\text{CCL}}}{dx} = \frac{-1.5}{6F}j_c\left(1 + 6n_d^{\text{MeOH}}\right) \tag{43}$$

Boundary conditions

Now that we have the models equations, boundary conditions for each one is needed. The variables in the model includes C_{MeOH}, $C_{H_2O_a}$, $C_{H_2O_c}$, C_{O_2}, ϕ_s, ϕ_l, i_l, i_s, u and p. Methanol and water concentration at cell entrance are written as [6]

$$C_{\text{MeOH}}^{fc,\text{in}} = A \tag{44}$$

$$C_{\text{MeOH}}^{fc,\text{in}} = \frac{\rho_{H_2O}}{M_{H_2O}}\left(1 - \frac{C_{\text{MeOH}}^{\text{in}} M_{\text{MeOH}}}{\rho_{\text{MeOH}}}\right) \tag{45}$$

Values of A, ρ_{H_2O}, M_{H_2O} are specified in table. 1. Inlet oxygen concentration is expressed using molar flowrate of oxygen and inlet pressure

$$C_{H_2O}^{fc,\text{in}} = x_{O_2}\frac{P_{ac,\text{in}}}{RT} \tag{46}$$

It was previously mentioned that all methanol is assumed to be consumed in CCL

$$C_{H_2O}^{fc,\text{in}} = x_{O_2}\frac{P_{ac,\text{in}}}{RT} \tag{47}$$

Boundary layer conditions for i_l are

$$i_l^{\text{ABL,ACL}} = 0 \qquad\qquad \text{at interface of ACL and ABL} \tag{48}$$

$$i_l = i_{\text{cell}} \qquad\qquad \text{at interface of ACL and M} \tag{49}$$

and boundary layer conditions for i_s are

$$i_s = i_{\text{cell}} + i_{\text{xover}} \tag{50}$$

$$i_s = 0 \tag{51}$$

For proton and electron transfer equation boundary conditions are

$$\phi_{s,FC/ABL} = 0 \qquad (52)$$

$$\phi_{s,CBL/AC} = V_{cell} \qquad (53)$$

3. Results and discussions

Consider a three-dimensional direct methanol fuel cell as illustrated in Figure.1. The simulated fuel cell includes a fluid channel, a backing layer, and a catalyst layer in both electrodes, and a membrane separator between the two electrodes. The cell structure materials are assumed as follows: Nafion 117 for membrane, carbon cloth for backing layers, Pt-black for CCl and Pt-Ru alloy for ACL. All other specifications and physiochemical properties are also given in Table. 1.
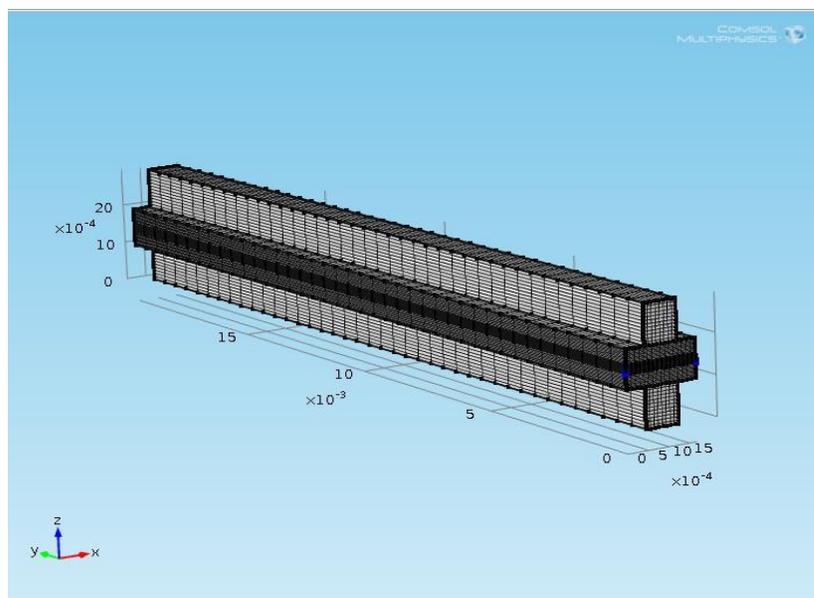
Figure. 1 Dimensions and geometry of simulated cell consisting of 37120 elements.

Table. 1 Geometrical and physiochemical parameters

Parameter	Notation	Value	Ref

Cell Length	l_{cell}	2×10^{-2} m	[8]

Table. 2 Geometrical and physiochemical parameters (continued)

Air and Fuel Channel Width	w_{ac}, w_{fc}	0.7874×10^{-3} m	[8]
Air and Fuel Channel Thickness	t_{ac}, t_{fc}	1×10^{-3} m	[8]
Diffusion Layers Thickness	t_B	3.8×10^{-4} m	[8]
Catalyst Layers Thickness	t_A	5×10^{-5} m	[8]
Polymer Membrane Thickness	t_M	1.83×10^{-4} m	[9]
Methanol concentration in fuel channel	C_{fc}^{MeOH}	2000 mol m^{-3}	[6]
Stoichiometric flow ratio of fuel channel	ζ_a	4	[6]
Stoichiometric flow ratio of air channel	ζ_c	4	[6]
Cell temperature	T	70	[6]
Pressure	P	1 atm	[6]
Dual Diffusion Coefficient of Methanol and Water	D_{MeOH, H_2O}	2.338×10^{-7} m^{2}s^{-1}	[10]
Dual Diffusion Coefficient of Liquid Water and Carbon Dioxide	D_{H_2O, C_2O}	5×10^{-10} m^{2}s^{-1}	[10]
Dual Diffusion Coefficient of Liquid Methanol and Carbon Dioxide	D_{MeOH, C_2O}	4.82×10^{-10} m^{2}s^{-1}	[10]
Dual Diffusion Coefficient of Oxygen and Steam	D_{O_2, H_2O}	3.405×10^{-5} m^{2}s^{-1}	[10]
Dual Diffusion Coefficient of Oxygen and Nitrogen	D_{O_2, N_2}	2.9×10^{-5} m^{2}s^{-1}	[10]

Dual Diffusion Coefficient of Nitrogen and Steam	D_{N_2,H_2O}	3.1×10^{-5} m^{2}s^{-1}	[10]

Table. 3 Geometrical and physiochemical parameters (continued)

Water Electro-Osmotic Drag Coefficient	$n_d^{H_2O}$	$1.6767 + 0.0155 \times T + 8.9074 \times 10^{-5} \times T^2$	[11]
Cell Voltage	V	0.4 V	[6]
Diffusion Layers Porosity	ε_B	0.4	[8]
Catalyst Layers Porosity	ε_A	0.3	[8]
Membrane Porosity	ε_M	0.3	[8]
Backing Layers Permeability	K_B	1.18×10^{-11} m^2	[12]
Catalyst Layers Permeability	K_A	2.36×10^{-12} m^2	[12]
Backing Layers Electric Conductivity	σ_B	222 S m^{-1}	[13]
Ion Membrane Conductivity	σ_m	9.825 S m^{-1}	[13]
Anode Transportation Coefficient	α_a	0.5	[6]
Cathode Transportation Coefficient	α_c	0.5	[6]
Anode Transfer Current Density in Standard Condition	j_{oa}^{ref}	1×10^5 A m^{-2}	[6]
Cathode Transfer Current Density in Standard Condition	j_{oc}^{ref}	1 A m^{-2}	[6]
Methanol Reference Concentration	C_{MeOH}^{ref}	100 mol m^{-3}	[6]
Oxygen Reference Concentration	$C_{O_2}^{ref}$	40.88 mol m^{-3}	[6]
Specific Area of the Active Surface	A_v	1×10^4 m^{-1}	[6]

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The predicted polarization given by the 3-D simulation is shown against experimental data in Figure. 2. As can be seen there is a good match between simulation results and that of Ge and Liu [8]. The highest current density in the curve is 2280 A m^{-2} located at 0.2 V and the cell is inoperable at lower voltages because current density becomes so high that concentration polarization drop occurs. At current densities 2280 A m^{-2} and higher, experiments show a divergence from linearity due to permeation limitations though in the present model it continues to be linear. The reason for which is that we have not taken into account the effects of two-phase flow.
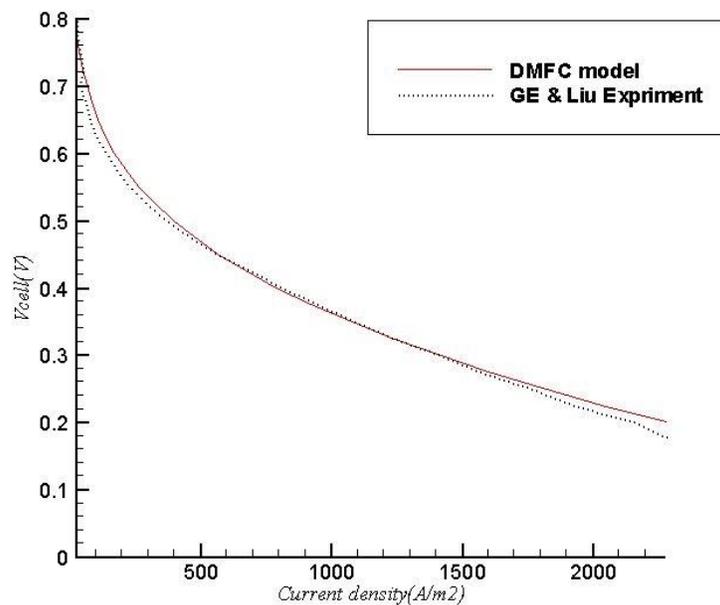
Figure. 2 Validation of present DMFC model against experimental data of Ge and liu

Methanol concentration distribution is shown for no crossover model in Figure. 3 and for crossover included model in Figure. 3. In both figures of Figure. 3 and Figure. 3 methanol concentration decreases from inlet to outlet and along thickness from fuel channel to ACL. When methanol crossover is not taken into account methanol consumption in reaction is the sole reason for depletion but when its effects are included we will also have a decrease in concentration due to diffusion and electro-osmosis. Detrimental effects of methanol crossover on methanol concentration can be seen in Figure. 3 and Figure. 3. It can be numerically seen that methanol concentration in cell outlet is 1350 mol m^{-3} when crossover is neglected and 1150 mol m^{-3} when we have methanol crossover.
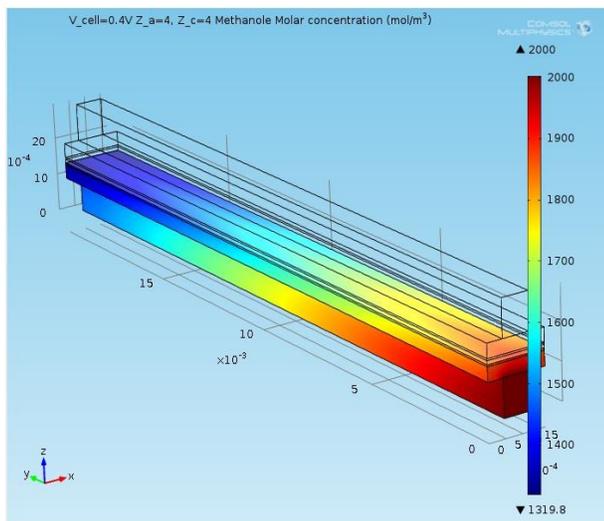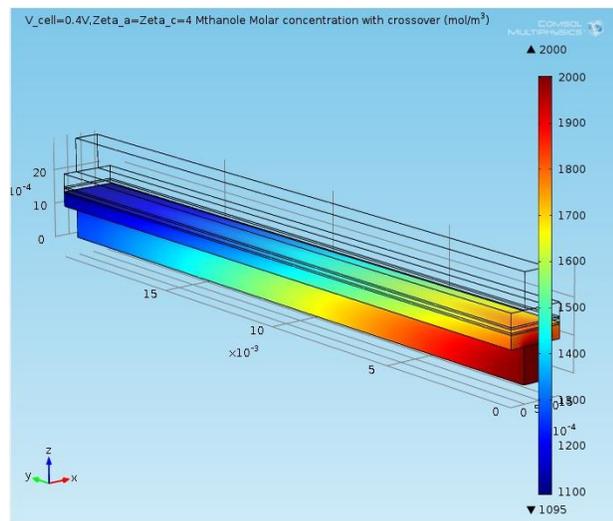
(a) without crossover model   (b) with crossover model

Figure. 3 methanol concentration distribution at $v_{cell} = 0.4$ v and $\zeta_a = \zeta_c = 4$

Oxygen concentration distribution for both with and without crossover models can be seen in figures Figure. 4 and Figure. 4b . As can be seen in both models oxygen concentration decreases from inlet to outlet and also in the direction of thickness from air channel to cathode catalyst layer. The reason for depletion in no crossover model is oxygen reduction reaction in CCL but in the model with crossover included it intensifies due to oxidation of methanol in CCL which is evident in the figures. Numerically speaking mean oxygen concentrations in cell exhaust in with crossover model and without crossover model respectively are 2.5 and 0.5 mol m^{-3}.

Figure. 5 andFigure. 6 corresponds to polarization and power density curves. Since anode volumetric current density is dependent on methanol concentration in anode and cathode volume current density is dependent on oxygen concentration in cathode, current density is lower when we consider crossover. Crossover decreases cell current density limit from 2280 A m^{-2} to 1142 A m^{-2}. It also decreases max cell power density from 456 W m^{-2} to 342.6 W m^{-2}.
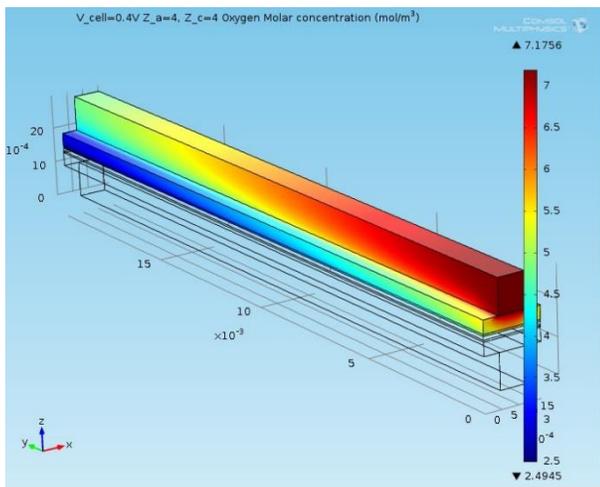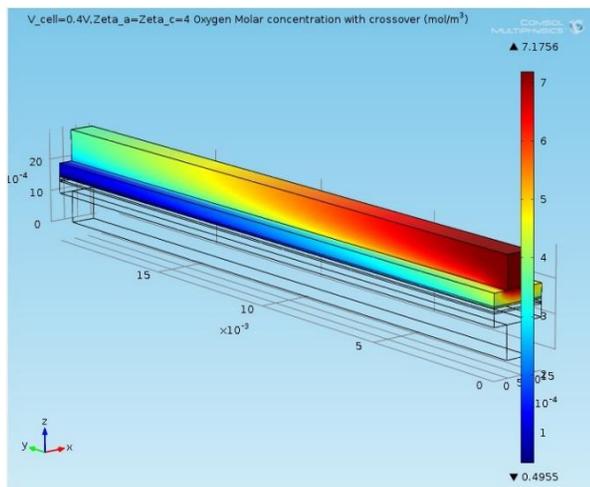
(a) without crossover model   (b) with crossover model

Figure. 4 oxygen concentration distribution at $v_{cell} = 0.4$ v and $\zeta_a = \zeta_c = 4$
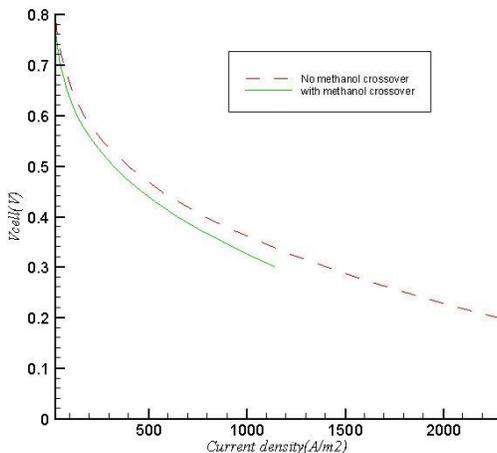
Figure. 5 Polarization of both models
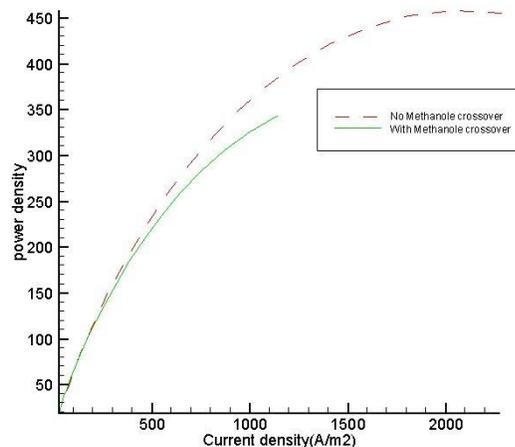
Figure. 6 Power density of both models

4. Conclusion

In the present paper we simulated direct methanol fuel cells using a CFD package. The governing equations of this kind of fuel cells includes equations such as conservation of mass,

momentum, charge and chemical species. Since these equations should be solved simultaneously which is very difficult, we used the COMSOL software. The layers are modeled in COMSOL and the results are presented.

Comparing the model with crossover to the one without crossover revealed that methanol crossover results in loss of reactants in both cathode and anode, which in turn lowers current and power densities. Crossover almost halved cell current density limit and decreased max power density by one fourth.

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