

Supplementary Materials for

Single and Double-sided Coated Gas Diffusion Layers used in Polymer Electrolyte Fuel Cells: A Numerical Study

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Source terms used in the transport equations:

1. Mass transport:

$S_{\text{mass}} = 0$. Where S_{mass} is the mass source term

2. Momentum transport:

$$S_{\text{mom}} = \frac{\mu \vec{u}}{K}$$

where S_{mom} is the momentum source, μ is the dynamic viscosity, \vec{u} is the velocity vector, and K is the permeability.

3. Species transport:

S_k is the source term that represents either consumption/production of species k (H_2 , O_2 or H_2O) and is given as follows [26, 27]:

$$S_{\text{H}_2} = -\frac{i_a a_a}{2F} M_{\text{H}_2}$$

$$S_{\text{O}_2} = -\frac{i_c a_c}{4F} M_{\text{O}_2}$$

$$S_{\text{H}_2\text{O}} = \frac{i_c a_c}{2F} M_{\text{H}_2\text{O}}$$

where i_a and i_c are the anodic and cathodic local current density respectively, a_a and a_c are the anodic and cathodic specific surface areas respectively, F is the Faraday's constant (96485 C/mol), and M_{H_2} , M_{O_2} and $M_{\text{H}_2\text{O}}$ are the molecular weights for hydrogen, oxygen and water respectively.

4. Energy transport:

S_e is the heat source term and takes one of the following forms in each fuel cell component [25]:

$$S_e = \begin{cases} i_s^2/\sigma_s \text{ for anode and cathode GDLs} \\ R_a \left[\eta_a - \frac{T\Delta S_a}{2F} \right] + \frac{i_s^2}{\sigma_s} + \frac{i_m^2}{\sigma_m} \text{ for anode catalyst layer} \\ R_c \left[-\eta_c - \frac{T\Delta S_c}{2F} \right] + \frac{i_s^2}{\sigma_s} + \frac{i_m^2}{\sigma_m} \text{ for cathode catalyst layer} \end{cases}$$

where R_a and R_c are the anode and cathode exchange current densities, i_s and i_m are the solid phase and membrane phase current densities, σ_s and σ_m are the electrical and ionic conductivities of the solid and membrane phases respectively, and η_a and η_c are the anodic and cathodic overpotential, ΔS_a and ΔS_c are the reaction entropies at anode and cathode catalyst layers respectively.

5. Charge transport:

$S_{\phi,s}$ and $S_{\phi,m}$ are the solid-phase potential and membrane-phase potential respectively and are given as follows [31]:

$$S_{\phi,s} = \begin{cases} j_a \text{ at the anode CL} \\ -j_c \text{ at the cathode CL} \end{cases}$$

$$S_{\phi,m} = \begin{cases} -j_a \text{ at the anode CL} \\ j_c \text{ at the cathode CL} \end{cases}$$

where j_a and j_c are the volumetric exchange current density (A/m^3) at the anode and cathode catalyst layers respectively and are obtained using Butler-Volmer equations [32]:

$$j_a = i_a^{\text{ref}} a_a \left(\frac{c_{H_2}}{c_{H_2}^{\text{ref}}} \right)^{0.5} \left[\exp \left(\frac{\alpha_{a,a} F}{RT} \eta_{\text{act},a} \right) - \exp \left(\frac{\alpha_{a,c} F}{RT} \eta_{\text{act},a} \right) \right]$$

$$j_c = i_c^{\text{ref}} a_c \left(\frac{c_{O_2}}{c_{O_2}^{\text{ref}}} \right) \left[\exp \left(\frac{\alpha_{c,a} F}{RT} \eta_{\text{act},c} \right) - \exp \left(\frac{\alpha_{c,c} F}{RT} \eta_{\text{act},c} \right) \right]$$

where i_a^{ref} and i_c^{ref} are the reference anodic and cathodic exchange current density respectively, $\alpha_{a,a}$ and $\alpha_{a,c}$ are respectively the anode and cathode transfer coefficients for the electrochemical reactions in the anode catalyst layer, $\alpha_{c,a}$ and $\alpha_{c,c}$ are respectively the anode and cathode transfer coefficients in the cathode catalyst layer, $c_{H_2}^{\text{ref}}$ and $c_{O_2}^{\text{ref}}$ are the reference hydrogen and oxygen concentrations respectively, F is the Faraday's constant and R is the universal gas constant. $\eta_{\text{act},a}$ and $\eta_{\text{act},c}$ are the anodic and cathodic overpotential and are given as follows:

$$\eta_{\text{act},a} = \phi_s - \phi_m$$

$$\eta_{\text{act},c} = \phi_s - \phi_m - E_0$$

where E_0 is the reference potential of the electrodes and is equal to zero for the anode, while for the cathode it is equal to the equilibrium cell potential (E_r) [33,34]:

$$E_r = 1.482 - 0.000845T + 0.0000431T \ln (P_{H_2} P_{O_2}^{0.5})$$

The membrane ionic conductivity, σ_m , is estimated using an empirical correlation developed by [35]:

$$\phi_m = (0.005139\lambda - 0.00326) \exp \left[1268 \left(\frac{1}{303} - \frac{1}{T} \right) \right]$$

where λ is the membrane water content which is empirically correlated by [32]:

$$\lambda = \begin{cases} 1.409 + 11.26ac - 18.77ac^2 + 16.21ac^3, & 0 < ac \leq 1 \\ 10.11 + 2.944(ac - 1), & 1 < ac \leq 3 \\ 16.8, & ac > 3 \end{cases}$$

where ac is the water activity and is given as [27]:

$$ac = \frac{P_v}{P_s}$$

where P_v is the partial pressure of water vapour and P_s is the pressure of saturated water vapor which is given by [27]:

$$\log(P_s) = -2.1794 + 0.02953(T - 273.15) - 9.1837 \times 10^{-5}(T - 273.15)^2 + 1.4454 \times 10^{-7}(T - 273.15)^3$$

6. Liquid water transport:

S_l is the source for the liquid phase, and is specified as follows [25]:

$$S_l = S_{\text{phase}} - S_\lambda M_{\text{H}_2\text{O}} + \frac{i_c}{2F} M_{\text{H}_2\text{O}} \text{ at the cathode catalyst layer.}$$

$S_l = S_{\text{phase}}$ at the anode catalyst layer, anode gas diffusion layer, and the cathode gas diffusion layer given as follows:

$$S_{\text{phase}} = \begin{cases} K_{\text{cond}} \frac{\varepsilon(1-s)x_v}{RT} M_{\text{H}_2\text{O}} (P_v - P_s) & P_v \geq P_s \\ K_{\text{evap}} \varepsilon \rho_l (P_v - P_s) & P_v < P_s \end{cases}$$

where K_{cond} is the rate of condensation, K_{evap} is the rate of evaporation, ρ_l is the density of liquid water, and x_v is the mole fraction of water vapour.

$$S_\lambda = \gamma_a \frac{\rho_m}{M_m} (\lambda^{\text{eq}} - \lambda) \text{ at the anode catalyst layer}$$

$$S_\lambda = \gamma_c \frac{\rho_m}{M_m} (\lambda^{\text{eq}} - \lambda) + \frac{i_c}{2F} \text{ at the cathode catalyst layer}$$

where ρ_m is the density of the dry membrane and M_m is the membrane equivalent weight.