USER MANUAL

The purpose of the model is to predict performance of a single cell, of which the geometric parameters, material properties, transport parameters and the operating conditions are specified by the user.

The capability of the model includes multiple flow field architectures (land-channel flow field or open flow field), flow arrangements (coflow or counterflow), oxidants (air or heliox). Important material and transport parameters (water content – activity correlation, ionic conductivity, dissolved water diffusion coefficient) can be tailored by user input.

Model validation can be done at performance and / or water balance level through trial and error procedure:

1. if performance is the only concern: voltage can be found by trial and error until the output current density matches the input target current density.
2. If water balance is concerned as well: in the case of coflow operation, follow the same procedure as finding out voltage; in the case of counterflow operation, it is suggested that voltage be found out first by trial and error and then the water flow rate at exit be found by trial and error until current density matches the input target current density and water molar flow rate matches the inlet flow rate by back-of-envelope calculation.

Three elements to run the program:

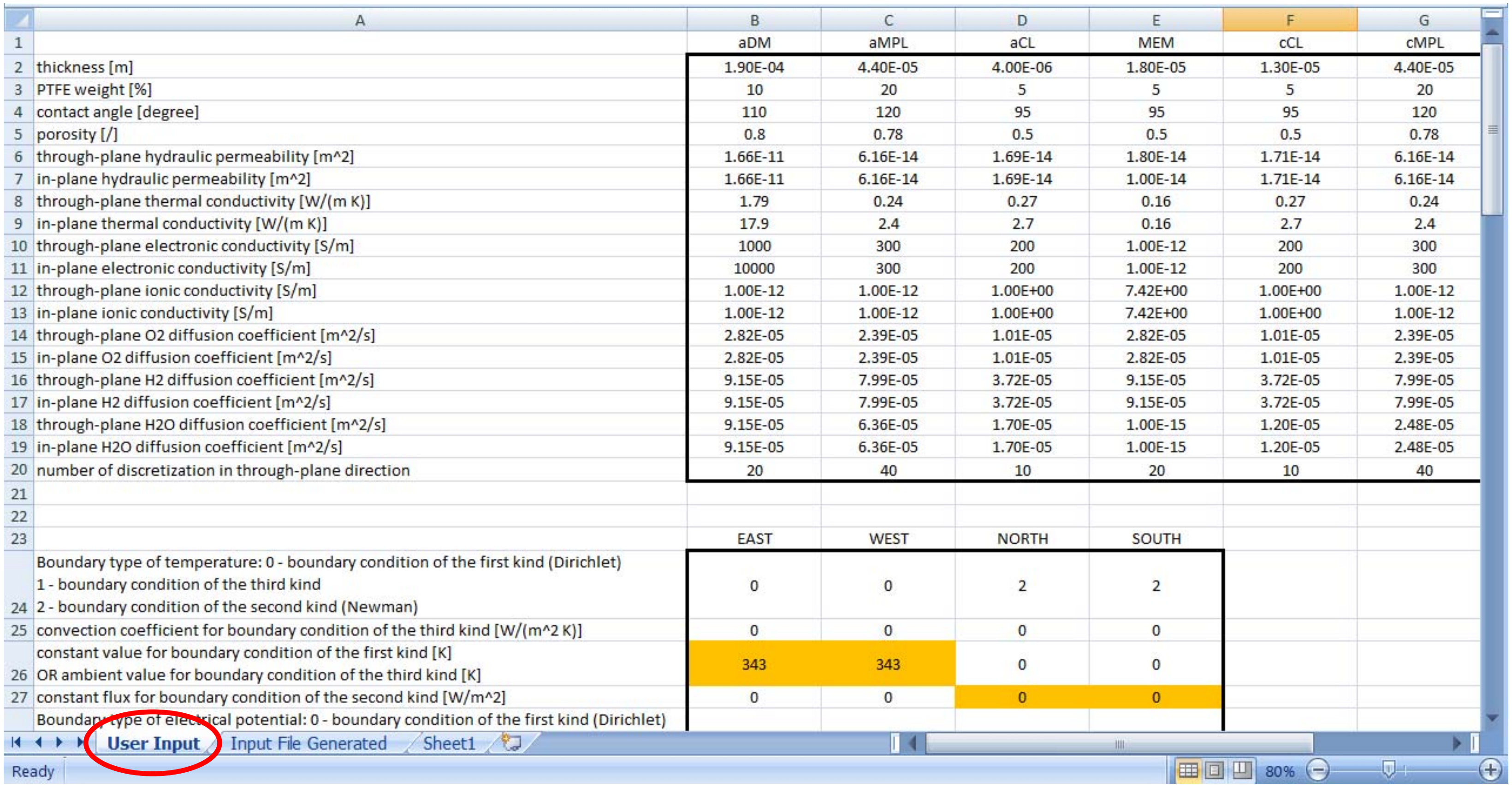
1. input file “input.dat” copied & pasted from input worksheet “input.xlsx”.
2. executable program “TEST.exe”.
3. an empty folder named “out”, where all the output files will be.

Steps to run the program:

1. prepared “input.dat” from “input.xlsx”
2. Make sure all “input.dat”, “TEST.exe” and folder “out” are under the same directory.
3. double click “TEST.exe”

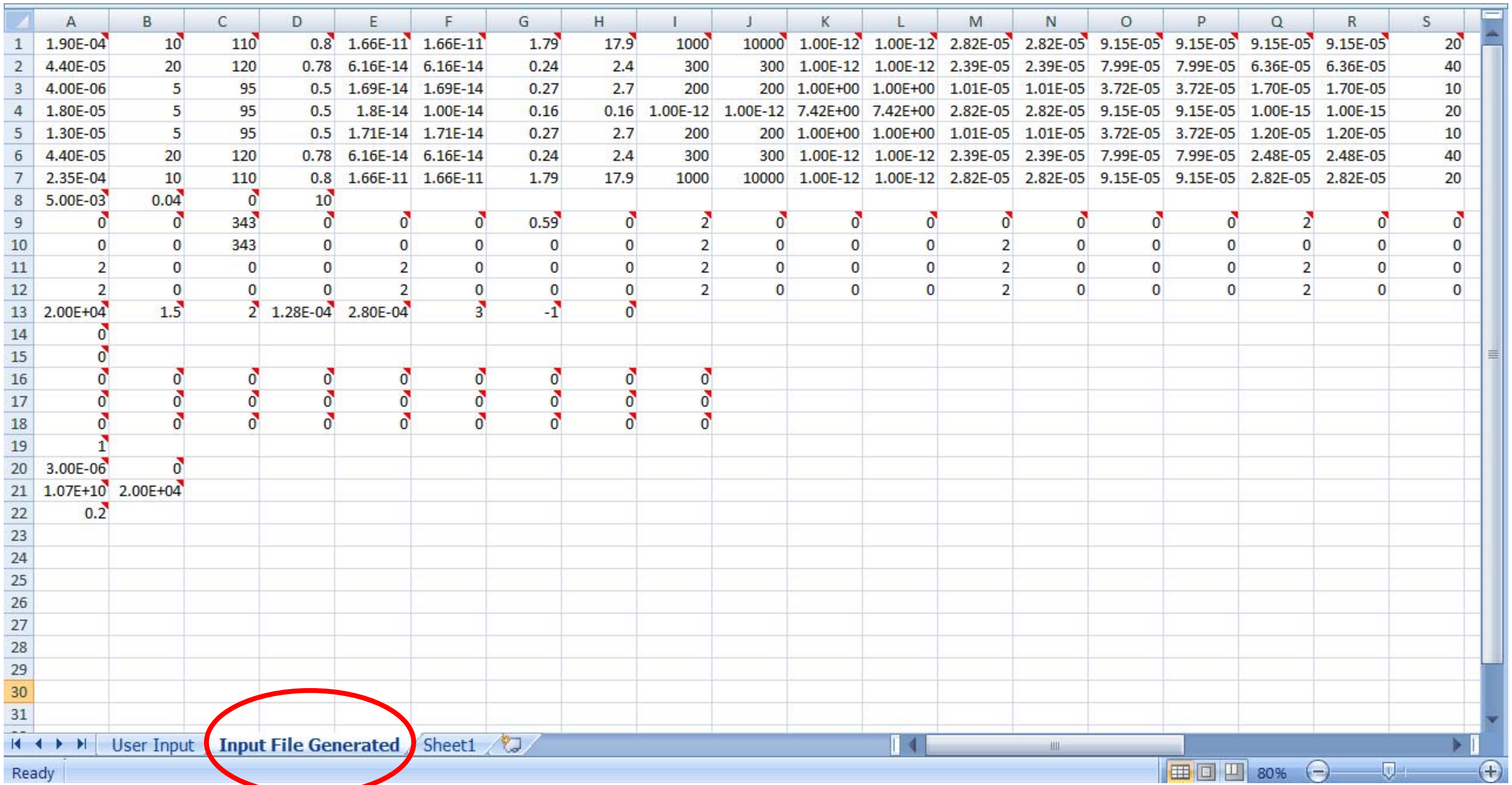
INPUT

The excel file "input.xlsx" is the input worksheet. The boxed region in "User Input" tab, as highlighted, is where user input is required.



	A	B	C	D	E	F	G
1		aDM	aMPL	aCL	MEM	cCL	cMPL
2	thickness [m]	1.90E-04	4.40E-05	4.00E-06	1.80E-05	1.30E-05	4.40E-05
3	PTFE weight [%]	10	20	5	5	5	20
4	contact angle [degree]	110	120	95	95	95	120
5	porosity [/]	0.8	0.78	0.5	0.5	0.5	0.78
6	through-plane hydraulic permeability [m^2]	1.66E-11	6.16E-14	1.69E-14	1.80E-14	1.71E-14	6.16E-14
7	in-plane hydraulic permeability [m^2]	1.66E-11	6.16E-14	1.69E-14	1.00E-14	1.71E-14	6.16E-14
8	through-plane thermal conductivity [W/(m K)]	1.79	0.24	0.27	0.16	0.27	0.24
9	in-plane thermal conductivity [W/(m K)]	17.9	2.4	2.7	0.16	2.7	2.4
10	through-plane electronic conductivity [S/m]	1000	300	200	1.00E-12	200	300
11	in-plane electronic conductivity [S/m]	10000	300	200	1.00E-12	200	300
12	through-plane ionic conductivity [S/m]	1.00E-12	1.00E-12	1.00E+00	7.42E+00	1.00E+00	1.00E-12
13	in-plane ionic conductivity [S/m]	1.00E-12	1.00E-12	1.00E+00	7.42E+00	1.00E+00	1.00E-12
14	through-plane O2 diffusion coefficient [m^2/s]	2.82E-05	2.39E-05	1.01E-05	2.82E-05	1.01E-05	2.39E-05
15	in-plane O2 diffusion coefficient [m^2/s]	2.82E-05	2.39E-05	1.01E-05	2.82E-05	1.01E-05	2.39E-05
16	through-plane H2 diffusion coefficient [m^2/s]	9.15E-05	7.99E-05	3.72E-05	9.15E-05	3.72E-05	7.99E-05
17	in-plane H2 diffusion coefficient [m^2/s]	9.15E-05	7.99E-05	3.72E-05	9.15E-05	3.72E-05	7.99E-05
18	through-plane H2O diffusion coefficient [m^2/s]	9.15E-05	6.36E-05	1.70E-05	1.00E-15	1.20E-05	2.48E-05
19	in-plane H2O diffusion coefficient [m^2/s]	9.15E-05	6.36E-05	1.70E-05	1.00E-15	1.20E-05	2.48E-05
20	number of discretization in through-plane direction	20	40	10	20	10	40
21							
22							
23		EAST	WEST	NORTH	SOUTH		
24	Boundary type of temperature: 0 - boundary condition of the first kind (Dirichlet) 1 - boundary condition of the third kind 2 - boundary condition of the second kind (Newman)	0	0	2	2		
25	convection coefficient for boundary condition of the third kind [W/(m^2 K)]	0	0	0	0		
26	constant value for boundary condition of the first kind [K] OR ambient value for boundary condition of the third kind [K]	343	343	0	0		
27	constant flux for boundary condition of the second kind [W/m^2]	0	0	0	0		
	Boundary type of electrical potential: 0 - boundary condition of the first kind (Dirichlet)						

The "Input File Generated" tab, as highlighted, is generated according to the information provided in "User Input" tab and locked.



	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S
1	1.90E-04	10	110	0.8	1.66E-11	1.66E-11	1.79	17.9	1000	10000	1.00E-12	1.00E-12	2.82E-05	2.82E-05	9.15E-05	9.15E-05	9.15E-05	9.15E-05	20
2	4.40E-05	20	120	0.78	6.16E-14	6.16E-14	0.24	2.4	300	300	1.00E-12	1.00E-12	2.39E-05	2.39E-05	7.99E-05	7.99E-05	6.36E-05	6.36E-05	40
3	4.00E-06	5	95	0.5	1.69E-14	1.69E-14	0.27	2.7	200	200	1.00E+00	1.00E+00	1.01E-05	1.01E-05	3.72E-05	3.72E-05	1.70E-05	1.70E-05	10
4	1.80E-05	5	95	0.5	1.8E-14	1.00E-14	0.16	0.16	1.00E-12	1.00E-12	7.42E+00	7.42E+00	2.82E-05	2.82E-05	9.15E-05	9.15E-05	1.00E-15	1.00E-15	20
5	1.30E-05	5	95	0.5	1.71E-14	1.71E-14	0.27	2.7	200	200	1.00E+00	1.00E+00	1.01E-05	1.01E-05	3.72E-05	3.72E-05	1.20E-05	1.20E-05	10
6	4.40E-05	20	120	0.78	6.16E-14	6.16E-14	0.24	2.4	300	300	1.00E-12	1.00E-12	2.39E-05	2.39E-05	7.99E-05	7.99E-05	2.48E-05	2.48E-05	40
7	2.35E-04	10	110	0.8	1.66E-11	1.66E-11	1.79	17.9	1000	10000	1.00E-12	1.00E-12	2.82E-05	2.82E-05	9.15E-05	9.15E-05	2.82E-05	2.82E-05	20
8	5.00E-03	0.04	0	10															
9	0	0	343	0	0	0	0.59	0	2	0	0	0	0	0	0	0	2	0	0
10	0	0	343	0	0	0	0	0	2	0	0	0	2	0	0	0	0	0	0
11	2	0	0	0	2	0	0	0	2	0	0	0	2	0	0	0	2	0	0
12	2	0	0	0	2	0	0	0	2	0	0	0	2	0	0	0	2	0	0
13	2.00E+04	1.5	2	1.28E-04	2.80E-04	3	-1	0											
14	0																		
15	0																		
16	0	0	0	0	0	0	0	0	0										
17	0	0	0	0	0	0	0	0	0										
18	0	0	0	0	0	0	0	0	0										
19	1																		
20	3.00E-06	0																	
21	1.07E+10	2.00E+04																	
22	0.2																		
23																			
24																			
25																			
26																			
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28																			
29																			
30																			
31																			

Then you can copy and paste the contents into “input.dat”, which is the input file required to run the program.

Tailorable input parameters include (all in SI units):

1. for each layer in the fuel cell sandwich: thickness, hydrophobicity (PTFE weight percentage or contact angle), porosity, through-plane and in-plane hydraulic permeability, through-plane and in-plane thermal conductivity, through-plane and in-plane electronic conductivity, through-plane and in-plane ionic conductivity, through-plane and in-plane O_2 diffusion coefficient, through-plane and in-plane H_2 diffusion coefficient, through-plane and in-plane H_2O diffusion coefficient, number of grids in through-plane direction
2. active area, in-plane width, land/channel width ratio, number of grids in in-plane direction

3. for east / west / north / south boundaries in the 2-D sub-model (see **Appendix A: Computational Domain**), boundary conditions are specified for solved-for variables: temperature, electric potential, ionic potential, O_2 concentration, H_2 concentration, H_2O concentration, gas pressure, and liquid pressure. Each boundary condition is specified by four numbers: boundary type (1st kind, 2nd kind or 3rd kind of boundary condition?) convection coefficient for 3rd kind of boundary condition constant value for 1st kind of boundary condition / ambient value for 3rd kind of boundary condition constant flux for 2nd kind of boundary condition
4. operating current density, stoichiometry of O_2, stoichiometry of H_2, molar flow rate of H_2O in cathode stream, molar flow rate of H_2O in anode stream, coolant temperature gradient, flow arrangement (counterflow or coflow?), oxidant (air or heliox?)
5. functional form of parameters:
    capillary pressure – liquid saturation correlation (0 – Leverett [1] / 1 – Kumbur [2])
    electro-osmotic drag coefficient (0 – Zawodzinski [3] / 1 – Springer [4])
    water content – water activity correlation
      0 – Weber [5]
      1 – customization: $\lambda = \left(x_0 + x_1 a + x_2 a^2 + x_3 a^3 + x_4 a^4 + x_5 a^5\right)\left[\frac{E_a}{R_u}\left(\frac{1}{T_{ref}} - \frac{1}{T}\right)\right]$
    ionic conductivity – water content correlation
      0 – Jiang [6]
      1 – customization: $\kappa = \left(x_0 + x_1 \lambda + x_2 \lambda^2 + x_3 \lambda^3 + x_4 \lambda^4 + x_5 \lambda^5\right)\left[\frac{E_a}{R_u}\left(\frac{1}{T_{ref}} - \frac{1}{T}\right)\right]$
    water diffusion coefficient in electrolyte phase with respect to chemical potential gradient – water content correlation
      0 – Weber [5]
      1 – customization: $D_{\mu_0} = \left(x_0 + x_1 \lambda + x_2 \lambda^2 + x_3 \lambda^3 + x_4 \lambda^4 + x_5 \lambda^5\right)\left[\frac{E_a}{R_u}\left(\frac{1}{T_{ref}} - \frac{1}{T}\right)\right]$
6. whether to consider thermo-osmotic drag?
   electrical contact resistance, thermal contact resistance
   exchange current density for HOR, exchange current density for ORR
   ionomer volume fraction in cathode catalyst layer

OUTPUT

- There is a summarizing file named “summary.out” to contain the information about temperature and water balance in each segment in the along-flow direction (y). The calculated average current density and HFR are listed in the end.

summary.out

```
segment = 0
```

Segment ID #

```
temperature                                    343.000000
Co2  molar flow rate                  =          0.000389
Ch2o molar flow rate cathode          =          0.000128
Ch2  molar flow rate                  =          0.000518
Ch2o molar flow rate anode            =          0.000330
```

Temperature and water molar flow rate information in corresponding segment

```
 Avg current                                =     20735.131700
 Avg EOD molar flow rate                    =         0.214905
 Avg TOD molar flow rate                    =         0.034483
 Avg diffusion molar flow rate              =        -0.129027
 Avg hydraulic molar flow rate              =        -0.028717
 Net water molar flow rate = EOD + TOD + Diffusive + Hydraulic
=
   0.214905 + 1 *    0.034483 +  -0.129027 +  -0.028717 =
0.091644
 Effective Drag Coefficient                 =         0.426438
 Total Ohmic resistance                     =         6.32e-06
 Total HFR                                  =         2.84e-06
```

Current density, net water transport across membrane, Ohmic resistance in corresponding segment (in SI units)

```
SUCCESS! SEE OUTPUT
GLOBAL CURRENT DENSITY  =  20342.286523
GLOBAL HFR = 5.13e-006
```

Global current density and HFR, averaged in along-flow direction (y)

- There are separate output files, named as “solved-for-variable_result.out”, for each solved-for variable (temperature T, electric potential Ve, ionic potential Vp, O_2 concentration Co2, H_2 concentration Ch2, H_2O concentration Ch2o, gas pressure Pgas, and liquid pressure Pliq). The five columns represent ① index in through-plane direction (z) ② index in in-plane direction (x) ③ coordinate in through-plane direction (z) ④ coordinate in in-plane direction (x) ⑤ value.

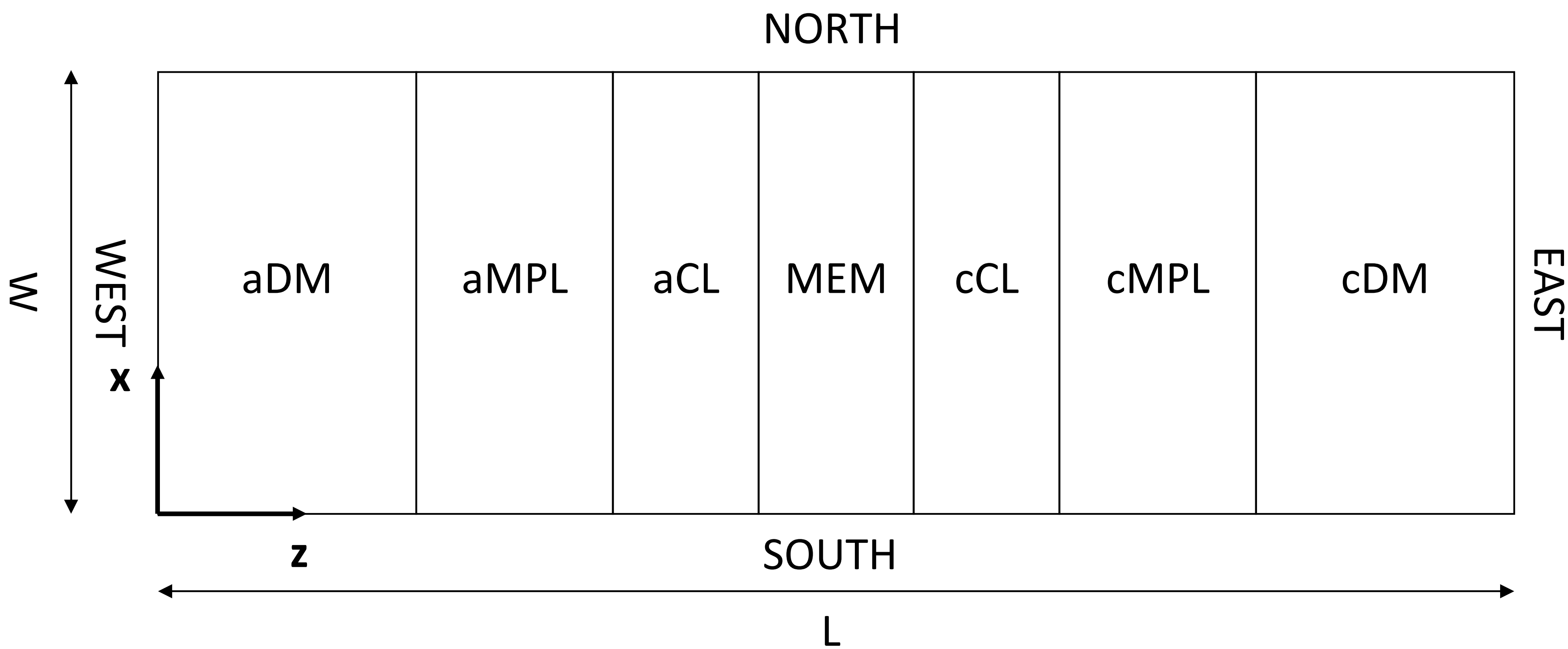
```
segment = 0
    1     1   0.000005   0.002000            343.015049
    2     1   0.000014   0.002000            343.045147
    3     1   0.000024   0.002000            343.075244
    4     1   0.000033   0.002000            343.105342
    5     1   0.000043   0.002000            343.135440
    6     1   0.000052   0.002000            343.165538
    7     1   0.000062   0.002000            343.195635
    8     1   0.000071   0.002000            343.225733
    9     1   0.000081   0.002000            343.255831
   10     1   0.000090   0.002000            343.285929
   11     1   0.000100   0.002000            343.316026
   12     1   0.000109   0.002000            343.346124
   13     1   0.000119   0.002000            343.376221
   14     1   0.000128   0.002000            343.406319
   15     1   0.000138   0.002000            343.436416
   16     1   0.000147   0.002000            343.466514
   17     1   0.000157   0.002000            343.496611
   18     1   0.000166   0.002000            343.526709
   19     1   0.000176   0.002000            343.556806
   20     1   0.000185   0.002000            343.586903
```

- There are separate output files, named as "flux_solved-for-variable_result.out", for the flux of each solved-for variable. The six columns represent ① index in through-plane direction (z) ② index in in-plane direction (x) ③ coordinate in through-plane direction (z) ④ coordinate in in-plane direction (x) ⑤ flux in through-plane direction (z) ⑥ flux in in-plane direction (x).

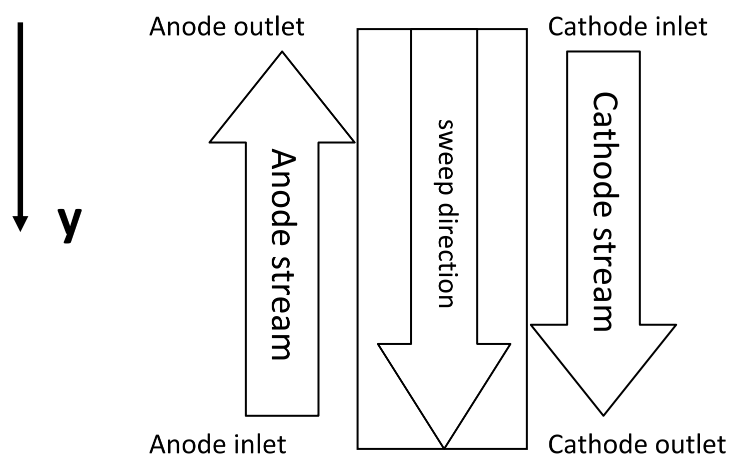
```
segment = 0
     1     1   0.000005   0.002000 -5660.081205  -0.000000
     2     1   0.000014   0.002000 -5660.080180  -0.000000
     3     1   0.000024   0.002000 -5660.078642  -0.000001
     4     1   0.000033   0.002000 -5660.076591  -0.000001
     5     1   0.000043   0.002000 -5660.074027  -0.000001
     6     1   0.000052   0.002000 -5660.070951  -0.000001
     7     1   0.000062   0.002000 -5660.067362  -0.000002
     8     1   0.000071   0.002000 -5660.063260  -0.000002
     9     1   0.000081   0.002000 -5660.058645  -0.000002
    10     1   0.000090   0.002000 -5660.053518  -0.000002
    11     1   0.000100   0.002000 -5660.047878  -0.000003
    12     1   0.000109   0.002000 -5660.041725  -0.000003
    13     1   0.000119   0.002000 -5660.035059  -0.000003
    14     1   0.000128   0.002000 -5660.027881  -0.000003
    15     1   0.000138   0.002000 -5660.020190  -0.000004
    16     1   0.000147   0.002000 -5660.011986  -0.000004
    17     1   0.000157   0.002000 -5660.003270  -0.000004
    18     1   0.000166   0.002000 -5659.994041  -0.000004
    19     1   0.000176   0.002000 -5659.984299  -0.000005
    20     1   0.000185   0.002000 -5659.973678  -0.000005
    21     1   0.000191   0.002000 -5659.961735  -0.000001
    22     1   0.000192   0.002000 -5659.948836  -0.000001
    23     1   0.000193   0.002000 -5659.935424  -0.000001
    24     1   0.000194   0.002000 -5659.921499  -0.000001
    25     1   0.000195   0.002000 -5659.907062  -0.000001
    26     1   0.000196   0.002000 -5659.892112  -0.000001
    27     1   0.000197   0.002000 -5659.876649  -0.000001
    28     1   0.000198   0.002000 -5659.860673  -0.000001
    29     1   0.000199   0.002000 -5659.844185  -0.000001
    30     1   0.000200   0.002000 -5659.827184  -0.000001
    31     1   0.000202   0.002000 -5659.809670  -0.000001
    32     1   0.000203   0.002000 -5659.791644  -0.000001
```

Appendix A: Computational Domain

2-D Sub-Model



+1 Simplification



Appendix B: Physics

- In porous media (including macro-porous GDL substrate, micro-porous layer, and catalyst layer)
  convective transport of gas species
  diffusive transport of gas species
  liquid water transport
  phase transfer between water vapor and liquid water
  convective transport of heat
  conductive transport of heat
  latent heat release / absorption by phase change
  electron transport
- In MEA (including catalyst layer and membrane)
  diffusive transport of dissolved water
  hydraulic permeation of water
  electro-osmosis
  thermo-osmosis
  conductive transport of heat
  Joule heating
  ion transport
- exclusive in catalyst layer
  hydrogen oxidation reaction
  oxygen reduction reaction
  phase transfer between water vapor / liquid water and dissolved water
  reversible and irreversible reaction heat release / absorption

Appendix C: Governing Equations

2-D sub-model

Parameter	Diffusion Media Micro-Porous Layer	Catalyst Layer	Membrane
C_{O_2}	$\vec{\nabla}\cdot\left(\vec{N}_{O_2,conv}\right)+\vec{\nabla}\cdot\left(\vec{N}_{O_2,diff}\right)=0$	$\vec{\nabla}\cdot\left(\vec{N}_{O_2,conv}\right)+\vec{\nabla}\cdot\left(\vec{N}_{O_2,diff}\right)=-\frac{J_{gen}}{4F}$	/
C_{H_2}	$\vec{\nabla}\cdot\left(\vec{N}_{H_2,conv}\right)+\vec{\nabla}\cdot\left(\vec{N}_{H_2,diff}\right)=0$	$\vec{\nabla}\cdot\left(\vec{N}_{H_2,conv}\right)+\vec{\nabla}\cdot\left(\vec{N}_{H_2,diff}\right)=-\frac{J_{gen}}{2F}$	/
C_{H_2O}	$\vec{\nabla}\cdot\left(\vec{N}_{H_2O,conv}\right)+\vec{\nabla}\cdot\left(\vec{N}_{H_2O,diff}\right)=-S_{vl}$	$\vec{\nabla}\cdot\left(\vec{N}_{H_2O,conv}\right)+\vec{\nabla}\cdot\left(\vec{N}_{H_2O,diff}\right)=-S_{vl}$	/
C_d	/	$\vec{\nabla}\cdot\left(-D_d\vec{\nabla}C_d\right)=-\vec{\nabla}\cdot\left(\alpha_{EOD}\frac{\vec{i}}{F}\right)-\vec{\nabla}\cdot\left(\alpha_{TOD}\vec{\nabla}T\right)+\frac{J_{gen}}{2F}$	$\vec{\nabla}\cdot\left(-D_d\vec{\nabla}C_d\right)=-\vec{\nabla}\cdot\left(\alpha_{EOD}\frac{\vec{i}}{F}\right)-\vec{\nabla}\cdot\left(\alpha_{TOD}\vec{\nabla}T\right)$
T	$\vec{\nabla}\cdot\left(\vec{q}_{conv}\right)+\vec{\nabla}\cdot\left(\vec{q}_{cond}\right)=\overline{H_{vl}}S_{vl}$	$\vec{\nabla}\cdot\left(\vec{q}_{conv}\right)+\vec{\nabla}\cdot\left(\vec{q}_{cond}\right)=S_T$ where $S_T=-J_{gen}(\eta+\frac{T\Delta S}{nF})+\frac{i^2}{\kappa}+\overline{H_{vl}}S_{vl}$	$\vec{\nabla}\cdot\left(\vec{q}_{cond}\right)=+\frac{i^2}{\kappa}$
P_G	$\vec{\nabla}\cdot\left(-C_T\frac{K_G}{\mu_G}\vec{\nabla}P_G\right)=-S_{vl}$	$\vec{\nabla}\cdot\left(-C_T\frac{K_G}{\mu_G}\vec{\nabla}P_G\right)=-\frac{J_{gen}}{nF}-S_{vl}$	/
P_L	$\vec{\nabla}\cdot\left(-\frac{\varepsilon_0 s\rho_W}{M_W}\frac{K_L}{\mu_L}\vec{\nabla}P_L\right)=S_{vl}$	$\vec{\nabla}\cdot\left(-\frac{\varepsilon_0 s\rho_W}{M_W}\frac{K_L}{\mu_L}\vec{\nabla}P_L\right)=S_{vl}$	$\vec{\nabla}\cdot\left(-\frac{\rho_W}{M_W}\frac{K_L}{\mu_L}\vec{\nabla}P_L\right)=0$
φ_e	/	$\vec{\nabla}\cdot\left(-\kappa\vec{\nabla}\varphi_e\right)=-J_{gen}$	$\vec{\nabla}\cdot\left(-\kappa\vec{\nabla}\varphi_e\right)=0$
φ_s	$\vec{\nabla}\cdot\left(-\sigma\vec{\nabla}\varphi_s\right)=0$	$\vec{\nabla}\cdot\left(-\sigma\vec{\nabla}\varphi_s\right)=J_{gen}$	/

$\vec{N}_{i,conv}=\vec{u}_G C_i$, where i=O_2, H_2, H_2O

$\nabla x_i=\sum_{j\neq i}\frac{x_i\vec{N}_{j,diff}-x_j\vec{N}_{i,diff}}{C_T D_{i,j}^{eff}}$, where i, j=O_2, H_2, H_2O

HOR: $J_{gen} = a i_{0,a}^{ref}(1-s)\left(\frac{C_{H_2}/H_{H_2,N}}{C_{H_2}^{ref}}\right)^{\gamma_a}\left[\exp\left(\frac{\alpha_{a,a}F}{R_u T}\eta\right)-\exp\left(\frac{-\alpha_{c,a}F}{R_u T}\eta\right)\right]$

ORR: $J_{gen} = 4F\left(\frac{C_{O_2}}{H_{O_2,N}}\right)^{\gamma_c}\left[\frac{1}{(1-\varepsilon_0^{CL})E_r k_c}+\frac{H_{O_2,W}}{H_{O_2,N}}\cdot\frac{\delta_W}{A_{agg}D_{O_2,W}}\cdot\frac{(r_{agg}+\delta_N)}{(r_{agg}+\delta_N+\delta_W)}+\frac{\delta_N}{A_{agg}D_{O_2,N}}\cdot\frac{(r_{agg}+\delta_N)}{r_{agg}}\right]^{-1}(1-s)$

$$S_{vl} = k_{vl}\left(C_{H_2O}RT - P_{sat}\right)$$

$$\vec{q}_{conv} = \left(\rho C_P \vec{u}\right)_G T + \left(\rho C_P \vec{u}\right)_L T$$

$$\vec{q}_{cond} = -k_{th}\vec{\nabla} T$$

$$\vec{u}_G = -\frac{K_G}{\mu_G}\nabla P_G$$

$$\vec{u}_L = -\frac{K_L}{\mu_L}\nabla P_L$$

+1 Simplification

$$\dot{n}_{H_2}^{k+1} = \dot{n}_{H_2}^{k} \mp \frac{i^k A^k}{2F}$$

$$\dot{n}_{O_2}^{k+1} = \dot{n}_{O_2}^{k} \mp \frac{i^k A^k}{4F}$$

$$\dot{n}_{N_2}^{k+1} = \dot{n}_{N_2}^{k}$$

$$\dot{n}_{H_2O,a}^{k+1} = \dot{n}_{H_2O,a}^{k} \mp \alpha_{net}^{k} \frac{i^k A^k}{F}$$

$$\dot{n}_{H_2O,c}^{k+1} = \dot{n}_{H_2O,c}^{k} \pm \left(\alpha_{net}^{k} + 0.5\right) \frac{i^k A^k}{F}$$

$$T^{k+1} = T^{k} \pm \frac{i^k A^k}{\dot{m} c_p} \left(E_{th} - E_{cell}\right)$$

Appendix D: Boundary Conditions

2-D sub-model

	1	2	3	4	5	6	7
	z=0	z=aMPL|aCL	z=aCL|PEM	z=MEM|cCL	z=cCL|cMPL	z=L	x=0 & x=W
C_{O_2}	/	/	/	$\nabla C_{O_2} = 0$	/	$C_{O_2} = C_{O_2}^{specified}$	$\nabla C_{O_2} = 0$
C_{H_2}	$C_{H_2} = C_{H_2}^{specified}$	/	$\nabla C_{H_2} = 0$	/	/	/	$\nabla C_{H_2} = 0$
C_{H_2O}	$C_{H_2O} = C_{H_2O}^{specified}$	/	/	/	/	$C_{H_2O} = C_{H_2O}^{specified}$	$\nabla C_{H_2O} = 0$
T	$T = T^{specified}$	/	/	/	/	$T = T^{specified}$	$\nabla T = 0$
P_G	$P_G = P_G^{specified}$	/	/	/	/	$P_G = P_G^{specified}$	$\nabla P_G = 0$
P_L	$P_L = P_L^{specified}$	/	/	/	/	$P_L = P_L^{specified}$	$\nabla P_L = 0$
φ_e	/	$\nabla \varphi_e = 0$	/	/	$\nabla \varphi_e = 0$	/	$\nabla \varphi_e = 0$
φ_s	$\varphi_s = \varphi^{specified}$	/	/	/	/	$\varphi_s = 0$	$\nabla \varphi_s = 0$

+1 Simplification

$$\dot{n}_{H_2}^{a,in} = \xi_{H_2} \frac{iA}{2F}$$

$$\dot{n}_{H_2O}^{a,in} = \dot{n}_{H_2}^{a,in} \times \frac{P_{sat}(T) \times RH}{P_a - P_{sat}(T) \times RH}$$

$$\dot{n}_{O_2}^{c,in} = \xi_{O_2} \frac{iA}{4F}$$

$$\dot{n}_{N_2}^{c,in} = \dot{n}_{O_2}^{c,in} \times \frac{79\%}{21\%} = \xi_{O_2} \frac{iA}{4F} \times \frac{79\%}{21\%}$$

$$\dot{n}_{H_2O}^{c,in} = \left(\dot{n}_{O_2}^{c,in} + \dot{n}_{N_2}^{c,in}\right) \times \frac{P_{sat}(T) \times RH}{P_c - P_{sat}(T) \times RH}$$

for the under-saturated gas flow in the flow field,

$$C_j^{a,k} = \frac{P_a}{R_u T^k} \frac{\dot{n}_j^{a,k}}{\dot{n}_{H_2}^{a,k} + \dot{n}_{H_2O}^{a,k}}$$ where j represents H_2 or H_2O

$$C_j^{c,k} = \frac{P_c}{R_u T^k} \frac{\dot{n}_j^{c,k}}{\dot{n}_{O_2}^{c,k} + \dot{n}_{N_2}^{c,k} + \dot{n}_{H_2O}^{c,k}}$$ where j represents O_2, N_2 or H_2O

for the saturated gas flow in the flow field,

$$C_j^{a/c,k} = \frac{P_{sat}(T^k)}{R_u T^k}$$ where j represents H_2O

$$C_j^{a,k} = \frac{P_a - P_{sat}\left(T^k\right)}{R_u T^k} \quad \text{where } j \text{ represents } H_2$$

$$C_j^{c,k} = \frac{P_c - P_{sat}\left(T^k\right)}{R_u T^k} \frac{\dot{n}_j^{c,k}}{\dot{n}_{O_2}^{c,k} + \dot{n}_{N_2}^{c,k}} \quad \text{where } j \text{ represents } O_2 \text{ or } N_2$$

Appendix E: Parameters

- reaction rate constant: reference [7]

$$k_c = \frac{a i_{0,c}^{ref}}{4F\left(C_{O_2}^{ref}\right)^{\gamma_c}} \exp\left(-\frac{\alpha_{c,c} F}{R_u T}\eta\right) \text{ [s}^{-1}\text{]}$$

- effectiveness factor: reference [7]

$$E_r = \frac{1}{\phi_L}\left(\frac{1}{\tanh(3\phi_L)} - \frac{1}{3\phi_L}\right) \text{ [/]}$$

- Thiele modulus: reference [7]

$$\phi_L = \frac{r_{agg}}{3}\sqrt{\frac{k_c}{D_{O_2,agg}^{eff}}} \text{ [/]}$$

- effective oxygen diffusion coefficient inside agglomerate: reference [8]

$$D_{O_2,agg}^{eff} = D_{O_2,N}\, {\varepsilon_N^{agg}}^{1.5} \text{ [m}^2\text{/s]}$$

- dissolved water concentration: defined

$$C_d = \frac{\rho_{dry}}{EW}\lambda \text{ [mol/m}^3\text{]}$$

- over-potential: defined

$\eta = \varphi_s - \varphi_e$ for HOR; $\eta = \varphi_s - \varphi_e - E_{rev}$ for ORR [V]

- catalyst loading: reference [manufacturer]

  L_a, L_c =0.15, 0.4 [mg_{Pt}/cm^2]

- accessible specific Pt surface area: reference [9]

  A_{Pt} =52.4 [$m^2{}_{Pt}/g_{Pt}$]

- roughness factor: reference [10]

  $$a_{a/c} = \frac{L_{a/c} A_{Pt}}{t_{aCL/cCL}} \text{ [m}^2{}_{Pt}\text{/m}^3\text{]}$$

- charge transfer coefficient: reference [11]

  $\alpha_{a,a}$, $\alpha_{c,a}$, $\alpha_{c,c}$ = 1, 1, 1 [/]

- reaction order: reference [11]

  γ_a, γ_c = 0.5, 1 [/]

- reference concentration: reference [11]

  $C^{ref}_{H_2/O_2}$ = 40 [mol/m^3]

- volumetric exchange current density

  ai_0^{ref} = $1.07 \cdot 10^{10}$ [A/m^3] for HOR, reference [12]

  ai_0^{ref} =fitting for ORR

- Henry's constant for oxygen into electrolyte: reference [13]

$$H_{O_2,N} = \frac{1.33\times10^5 \exp\left(-666/T\right)}{RT} \text{ [/]}$$

- Henry's constant for hydrogen into electrolyte: reference [13]

$$H_{H_2,N} = \frac{4.56\times10^3}{RT} \text{ [/]}$$

- Henry's constant for oxygen into liquid water: reference [14]

$$H_{O_2,W} = \frac{5.08\times10^5 \exp\left(-500/T\right)}{RT} \text{ [/]}$$

- agglomerate particle radius: reference [10, 15]

r_{agg} =0.5·10^{-6} [m]

- ionomer volume fraction inside agglomerate particle: reference [15]

ε_N^{agg} =0.5 [/]

- thickness of ionomer thin film surrounding agglomerate particle: reference [15]

δ_N =5·10^{-8} [m]

- thickness of water thin film surrounding agglomerate particle: reference [16]

$$\delta_W = \frac{\varepsilon_0^{CL} s}{A_{agg}} \text{ [m]}$$

- effective surface area for oxygen to dissolve into agglomerate particle: reference [16]

$$A_{agg} = \frac{3\left(1-\varepsilon_0^{CL}\right)}{\left(r_{agg}+\delta_N\right)}$$ [m^{-1}]

- oxygen diffusion coefficient in ionomer: reference [17]

$$D_{O_2,N} = 2.88\times10^{-10}\exp\left[2933\left(\frac{1}{313}-\frac{1}{T}\right)\right]$$ [m^2/s]

- oxygen diffusion coefficient in liquid water: reference [16]

$D_{O_2,W}$ =2.41·10^{-9} [m^2/s]

- water content λ ~ water activity a correlation: reference [5]

$$\left\{\begin{array}{l}
\frac{\lambda_{H_3O^+}}{\left(1-\lambda_{H_3O^+}\right)\left(\lambda-\lambda_{H_3O^+}\right)}\exp\left[\phi_1\lambda_{H_3O^+}\right]\exp\left[\phi_2\lambda\right]=K_1\\
a = K_2\left(\lambda-\lambda_{H_3O^+}\right)\exp\left[\phi_2\lambda_{H_3O^+}\right]\exp\left[\phi_3\lambda\right]\\
K_1 = 100\\
K_2 = 0.217\\
\phi_1 = \frac{2}{EW}\left(E_{0,0}^* - 2E_{H_3O^+,H^+}^* - 2E_{0,H_3O^+}^*\right)\\
\phi_2 = \frac{2}{EW}\left(E_{0,H_3O^+}^* - E_{0,0}^*\right)\\
\phi_3 = \frac{2E_{0,0}^*}{EW}\\
E_{0,0}^* = -41.7[g/mol]\\
E_{0,H_3O^+}^* = -52.0[g/mol]\\
E_{H_3O^+,H^+}^* = -3721.6[g/mol]
\end{array}\right.$$

- diffusion coefficient of dissolved water with regard to chemical potential gradient: reference [5]

$$D_{\mu_0} = 1.8\times10^{-9}\, f_V \exp\left[\frac{20000}{R}\left(\frac{1}{303}-\frac{1}{T}\right)\right]$$, where $f_V = \dfrac{\lambda\overline{V_0}}{\overline{V_m}+\lambda\overline{V_0}}$ [m^2/s]

- diffusion coefficient of dissolved water with regard to concentration gradient: reference [18]

$$D_d = D_{\mu_0}\left[\frac{d(\ln a)}{d(\ln\lambda)}\right]$$ [m^2/s]

- electro-osmotic drag coefficient: reference [3]

$$\alpha_{EOD} = \begin{cases} 1.0 & \lambda \le 14 \\ 2.5 & \lambda \ge 22 \end{cases}$$ [/]

- electro-osmotic drag coefficient: reference [4]

$$\alpha_{EOD} = \frac{2.5\lambda}{22}$$ [/]

- ionic conductivity in membrane , reference [6]

$$\kappa = 12\times RH^{1.67}\exp\left[\frac{12000}{R}\left(\frac{1}{353}-\frac{1}{T}\right)\right]$$ [S/m]

- ionic conductivity in cathode catalyst layer, [19]

$$\kappa = 3\times\varepsilon_N^{CL}\times12\times RH^{1.67}\exp\left[\frac{12000}{R}\left(\frac{1}{353}-\frac{1}{T}\right)\right]$$ [S/m]

- thermo-osmotic drag coefficient, reference [20]

$$\alpha_{TOD} = 9.22\times10^{-4}\exp\left[-\frac{2298}{T}\right]$$ [mol/m·s·K]

- Knudsen diffusion coefficient, reference [21]

$$D_{Kn} = \frac{4r_p}{3}\sqrt{\frac{2R_uT}{\pi M}} \text{ [m}^2\text{/s]}$$

- effective binary diffusion coefficient, reference [8, 21]

$$D_{i,j}^{eff} = \frac{[\varepsilon_0(1-s)]^{1.5} D_{i,j} D_{Kn}}{[\varepsilon_0(1-s)]^{1.5} D_{i,j} + D_{Kn}} [\varepsilon_0(1-s)]^{1.5} \text{ [m}^2\text{/s]}$$

- saturation pressure: reference [22]

$$P_{sat} = -2846.4 + 411.24T - 10.554T^2 + 0.16636T^3 \text{ [Pa], T in }^\circ\text{C}$$

- water activity: defined

$$a = \frac{C_{H_2O} R_u T}{P_{sat}} \text{ [/]}$$

- capillary pressure ~ liquid saturation correlation, reference [2]

$$P_{cap} = \gamma\left(\frac{\varepsilon_0}{K_0}\right)^{1/2}\left\{(wt\%)\left[0.0469 - 0.00152(wt\%) - 0.0406s^2 + 0.143s^3\right] + 0.0561\ln(s)\right\} \text{ [Pa]}$$

- capillary pressure ~ liquid saturation correlation, reference [1]

$$P_{cap} = \gamma\cos\theta\left(\frac{\varepsilon_0}{K_0}\right)^{1/2} J(s) \text{ [Pa]}$$

$$J(s) = \begin{cases} 1.417(1-s) - 2.120(1-s)^2 + 1.263(1-s)^3 & if\ \theta < 90^\circ \\ 1.417s - 2.120s^2 + 1.263s^3 & if\ \theta > 90^\circ \end{cases}$$

- effective permeability: defined

$K = K_0 K_r$ [m^2]

- relative permeability, reference [23]

$K_r = s_{nw}{}^{2.16}$ for non-wetting phase, $K_r = (1 - s_{nw})^{2.16}$ for wetting phase [/]

- entropy change of reaction: reference [24]

ΔS =0.104 for HOR [J/mol·K]

ΔS =-326.36 for ORR [J/mol·K]

- binary diffusion coefficient between water vapor and oxygen: reference [25]

D_{O_2,H_2O}, D_{H_2O,O_2} =2.82$\times$ 10^{-5} [m^2/s]

- binary diffusion coefficient between water vapor and nitrogen: reference [25]

D_{N_2,H_2O}, D_{H_2O,N_2} =2.93$\times$ 10^{-5} [m^2/s]

- binary diffusion coefficient between oxygen and nitrogen: reference [25]

D_{O_2,N_2}, D_{N_2,O_2} =2.30$\times$ 10^{-5} [m^2/s]

- binary diffusion coefficient between water vapor and helium: reference [25]

D_{He,H_2O}, $D_{H_2O,He}$ =9.08$\times$ 10^{-5}[m^2/s]

- binary diffusion coefficient between oxygen and helium: reference [25]

$D_{O_2,He}$, D_{He,O_2} =8.22$\times$ 10^{-5} [m^2/s]

- binary diffusion coefficient between hydrogen and water vapor: reference [25]

  D_{H_2,H_2O}, D_{H_2O,H_2} =9.15$\times$ 10^{-5} [m^2/s]

- density of dry membrane: reference [26]

  ρ_{dry} =1980 [kg/m^3]

- equivalent weight of membrane: reference [manufacturer]

  EW =1.1 [kg/equiv]

- ionomer volume fraction in cathode catalyst layer: reference [19]

  ε_N^{CL} =0.2 [/]

- density of liquid water: reference [27]

  ρ_W =10^3 [kg/m^3] ,

- molecular weight of water: reference [27]

  M_W =18·10^{-3} [kg/mol]

- dynamic viscosity: reference [27]

  μ = 3.65$\times$ 10^{-4} for liquid, 1.5$\times$ 10^{-5} for gas [Pa·s]

- molar latent heat of vaporization: reference [27]

  $\overline{H}_{vl}$ =40.65$\times$ 10^3 [J/mol]

- surface tension: reference [27]

γ=0.0625 [N/m]

- thermal voltage: reference [22]

E_{th} =1.25 [V]

- reversible voltage, reference [11]

$$E_{rev} = 1.23 - 0.9 \times 10^{-3}(T - 298) + 2.303\frac{R_u T}{4F} \times \log\left[\left(\frac{P_{H_2}}{P_{H_2}^*}\right)^2\left(\frac{P_{O_2}}{P_{O_2}^*}\right)\right] \text{ [V]}$$

- universal gas constant: reference [27]

R_u =8.314 [J/mol·K]

- Faraday constant

F =96485 [C/mol]

Appendix F: Reference

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