

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		
28	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																			
27																			
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 O₂ diffusion coefficient, through-plane and in-plane H₂ diffusion coefficient, through-plane and in-plane H₂O 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, O₂ concentration, H₂ concentration, H₂O 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 O₂, stoichiometry of H₂, molar flow rate of H₂O in cathode stream, molar flow rate of H₂O 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, O₂ concentration Co₂, H₂ concentration Ch₂, H₂O concentration Ch_{2o}, gas

pressure P_{gas} , and liquid pressure P_{liq}). 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).

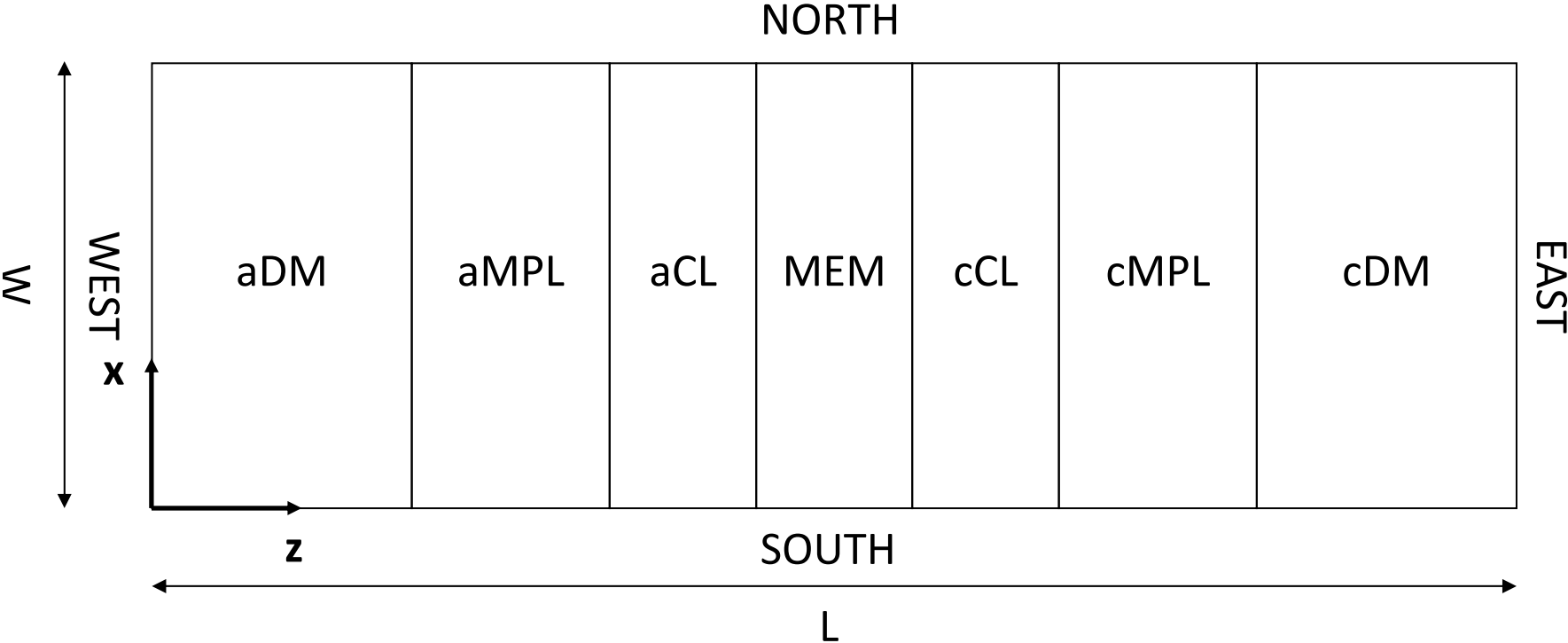
```

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

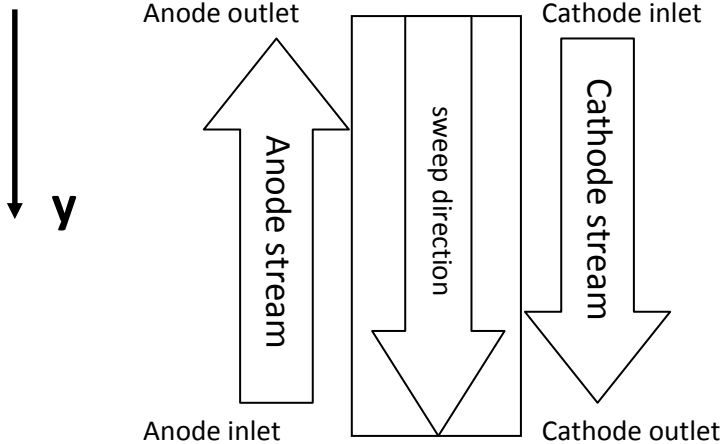
```

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

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

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

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

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

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

$$\bar{q}_{conv} = (\rho C_p \bar{u})_G T + (\rho C_p \bar{u})_L T$$

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

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

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

+1 Simplification

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

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

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

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

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

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

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	$\varphi_s = \varphi_s^{specified}$	/	/	/	/	$\varphi_s = 0$	$\nabla \varphi_s = 0$

+1 Simplification

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

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

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

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

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

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

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

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

for the saturated gas flow in the flow field,

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

$$C_j^{a,k} = \frac{P_a - P_{sat}(T^k)}{R_u T^k} \quad \text{where } j \text{ represents H}_2$$

$$C_j^{c,k} = \frac{P_c - P_{sat}(T^k)}{R_u T^k} \frac{\dot{n}_j^{c,k}}{\dot{n}_{O_2}^{c,k} + \dot{n}_{N_2}^{c,k}} \quad \text{where } j \text{ represents O}_2 \text{ or N}_2$$

Appendix E: Parameters

- reaction rate constant: reference [7]

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

- effectiveness factor: reference [7]

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

- Thiele modulus: reference [7]

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

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

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

- dissolved water concentration: defined

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

- over-potential: defined

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

- catalyst loading: reference [manufacturer]

$$L_a, L_c = 0.15, 0.4 \text{ [mg}_{Pt}/\text{cm}^2]$$

- accessible specific Pt surface area: reference [9]

$$A_{Pt} = 52.4 \text{ [m}^2_{Pt}/\text{g}_{Pt}]$$

- roughness factor: reference [10]

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

- charge transfer coefficient: reference [11]

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

- reaction order: reference [11]

$$\gamma_a, \gamma_c = 0.5, 1 \text{ []}$$

- reference concentration: reference [11]

$$C_{H_2/O_2}^{ref} = 40 \text{ [mol}/\text{m}^3]$$

- volumetric exchange current density

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

$$ai_0^{ref} = \text{fitting for ORR}$$

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

$$H_{O_2,N} = \frac{1.33 \times 10^5 \exp(-666/T)}{RT} \quad [l]$$

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

$$H_{H_2,N} = \frac{4.56 \times 10^3}{RT} \quad [l]$$

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

$$H_{O_2,W} = \frac{5.08 \times 10^5 \exp(-500/T)}{RT} \quad [l]$$

- agglomerate particle radius: reference [10, 15]

$$r_{agg} = 0.5 \cdot 10^{-6} \text{ [m]}$$

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

$$\varepsilon_N^{agg} = 0.5 \quad [l]$$

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

$$\delta_N = 5 \cdot 10^{-8} \text{ [m]}$$

- 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]

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

- oxygen diffusion coefficient in ionomer: reference [17]

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

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

$$D_{O_2,W} = 2.41 \cdot 10^{-9} [\text{m}^2/\text{s}]$$

- water content $\lambda \sim$ water activity a correlation: reference [5]

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

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

$$D_{\mu_0} = 1.8 \times 10^{-9} f_V \exp\left[\frac{20000}{R}\left(\frac{1}{303} - \frac{1}{T}\right)\right], \text{ where } f_V = \frac{\lambda \bar{V}_0}{V_m + \lambda \bar{V}_0} \text{ [m}^2/\text{s]}$$

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

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

- electro-osmotic drag coefficient: reference [3]

$$\alpha_{EOD} = \begin{cases} 1.0 & \lambda \leq 14 \\ 2.5 & \lambda \geq 22 \end{cases} \text{ [I]}$$

- electro-osmotic drag coefficient: reference [4]

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

- ionic conductivity in membrane , reference [6]

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

- ionic conductivity in cathode catalyst layer, [19]

$$\kappa = 3 \times \varepsilon_N^{CL} \times 12 \times RH^{1.67} \exp\left[\frac{12000}{R}\left(\frac{1}{353} - \frac{1}{T}\right)\right] \text{ [S/m]}$$

- thermo-osmotic drag coefficient, reference [20]

$$\alpha_{TOD} = 9.22 \times 10^{-4} \exp\left[-\frac{2298}{T}\right] \text{ [mol/m}\cdot\text{s}\cdot\text{K]}$$

- Knudsen diffusion coefficient, reference [21]

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

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

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

- saturation pressure: reference [22]

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

- water activity: defined

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

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

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

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

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

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

- effective permeability: defined

$$K = K_0 K_r \text{ [m}^2\text{]}$$

- relative permeability, reference [23]

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

- entropy change of reaction: reference [24]

$$\Delta S = 0.104 \text{ for HOR [J/mol}\cdot\text{K]}$$

$$\Delta S = -326.36 \text{ for ORR [J/mol}\cdot\text{K]}$$

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

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

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

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

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

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

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

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

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

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

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

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

- density of dry membrane: reference [26]

$$\rho_{dry} = 1980 \text{ [kg/m}^3\text{]}$$

- equivalent weight of membrane: reference [manufacturer]

$$EW = 1.1 \text{ [kg/equiv]}$$

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

$$\varepsilon_N^{CL} = 0.2 \text{ []}$$

- density of liquid water: reference [27]

$$\rho_W = 10^3 \text{ [kg/m}^3\text{]} ,$$

- molecular weight of water: reference [27]

$$M_W = 18 \cdot 10^{-3} \text{ [kg/mol]}$$

- dynamic viscosity: reference [27]

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

- molar latent heat of vaporization: reference [27]

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

- surface tension: reference [27]

$$\gamma = 0.0625 \text{ [N/m]}$$

- thermal voltage: reference [22]

$$E_{th} = 1.25 \text{ [V]}$$

- 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]

$$R_u = 8.314 \text{ [J/mol}\cdot\text{K]}$$

- Faraday constant

$$F = 96485 \text{ [C/mol]}$$

Appendix F: Reference

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