

Supporting Information for

**Electrode Informatics Accelerated Optimization for Catalyst
Layer Key Parameters in Direct Methanol Fuel Cells**

Lishou Ban^{a†}, Danyang Huang^{a†}, Yanyi Liu^{a†}, Pengcheng Liu^a, Xihui Bian^b, Kaili Wang^c, Yifan Liu^{*d}, Xijun Liu^{e*}, and Jia He^{a*}

a. School of Chemistry and Chemical Engineering, Institute for New Energy Materials & Low-Carbon Technologies, School of Materials Science and Engineering, Tianjin University of Technology, Tianjin 300384, China

b. State Key Laboratory of Separation Membranes and Membrane Processes, School of Chemical Engineering and Technology, Tiangong University, Tianjin 300387, China

c. School of Chemistry, Chemical Engineering and Environmental Engineering, Weifang University, Weifang 261061, China

d. Suzhou Laboratory, Suzhou 215100, China.

e. State Key Laboratory of Featured Metal Materials and Life-cycle Safety for Composite Structures, Guangxi Key Laboratory of Processing for Non-ferrous Metals and Featured Materials, School of Resources, Environment and Materials, Guangxi University, Nanning, 530004 Guangxi, China

† These authors contributed equally to this work.

* E-mail: sparkle06@163.com; xjliu@gxu.edu.cn; hejia1225@126.com

Table S1. Boundary conditions.

Boundary areas	Boundary conditions		
	Charge transport	Momentum transmission	Mass transport
Fuel inlet	-	U_in_anode	C _{MeOH_in} , 1M H ₂ O, 1e-4 M CO ₂
Fuel outlet	-	1 atm	Convection
Air inlet	-	U_in_cathode	xO _{2c_in} , xH ₂ O _{c_in}
Air outlet	-	1 atm	Convection
Anode GDL outer surface	Insulation	-	No slippage
Cathode GDL outer surface	Insulation	-	No slippage
Fuel and air flow channel walls	Insulation	No slippage	No slippage
Anode electrode outer surface	Electrical grounding	-	-
Cathode electrode outer surface	E _{cell}	-	-

Table S2. DMFC Model Parameters.

Parameter	Value
Runner length	0.01 m
Runner height	0.001 m
Runner width	1.5748E-4 m
Runner spacing	1.81864E-4 m
GDL height	3.8E-4 m
Porous electrode height	5E-5 m
Proton exchange membrane height	1E-4 m
Porosity of GDL	0.7
Permeability of GDL	1E-12 m ²
Electronic conductivity of GDL	222 S/m
Integral of the ionomer in CL	0.25
Porosity of CL	0.3
Permeability of CL	2E-14 m ²
Proton Conductivity of CL (nafion)	12.3 S/m
Electronic conductivity of CL (solid)	222 S/m
Conductivity of the membrane	9.825 S/m
Cathode oxygen mass fraction	0.228
Cathode water mass fraction	0.01
Molar mass of water	0.018 kg/mol
Molar mass of oxygen	0.032 kg/mol
Molar mass of nitrogen	0.028 kg/mol
Molar mass of cathode oxygen	0.20418
Molar mass of cathode water	0.015921
Molar mass of cathode nitrogen	0.77989
Anode inlet velocity	0.13 m/s
Cathode inlet velocity	0.4 m/s
Anode viscosity coefficient	1.19E-5 Pa·s
Cathode viscosity coefficient	2.46E-5 Pa·s
MeOH-H ₂ O Binary diffusion coefficient	1E-5 m ² /s
O ₂ -N ₂ Binary diffusion coefficient	2.8238E-5 m ² /s
O ₂ -H ₂ O Binary diffusion coefficient	3.3188E-5 m ² /s
N ₂ -H ₂ O Binary diffusion coefficient	3.0291E-5 m ² /s
Cell temperature	338.15 K
Reference pressure	1.01E5 Pa
Cell voltage	1 V
Oxygen reference concentration	36.5 mol/m ³
Methanol reference concentration	100 mol/m ³
Molar gas constant	8.314 J/(mol·K)
Specific surface area	1E5 1/m
Anode equilibrium potential	0.046 V
Cathode equilibrium potential	1.05 V
Anode reference current density	43.82 A/m ²
Cathode reference current density	0.0422 A/m ²
Inlet methanol concentration	1000 mol/m ³
Diffusion coefficient of methanol in the membrane	1.1989E-12 m ² /s

Table S3. DMFC Database

No.	T	thickness	thickness	poro	CL	poro	CL	enafion	CL	enafion	CL	elec	CL	elec	CL	in	U	in	ca	kappa	CL	kappa	CL	MeOH	in	Av	an	Av	ca	p_ref	sigma	CL	sigma	CL	MeOH	ref	2	FO
0	45	0.0005	0.0005	0.3	0.3	0.25	0.25	0.45	0.45	0.13	0.4	2.00E-14	2.00E-14	1	100000	100000	1	222	12.3	100	36.5	0.0572566																
1	55	0.0005	0.0005	0.3	0.3	0.25	0.25	0.45	0.45	0.13	0.4	2.00E-14	2.00E-14	1	100000	100000	1	222	12.3	100	36.5	0.0613302																
2	65	0.0005	0.0005	0.3	0.3	0.25	0.25	0.45	0.45	0.13	0.4	2.00E-14	2.00E-14	1	100000	100000	1	222	12.3	100	36.5	0.0636062																
3	75	0.0005	0.0005	0.3	0.3	0.25	0.25	0.45	0.45	0.13	0.4	2.00E-14	2.00E-14	1	100000	100000	1	222	12.3	100	36.5	0.0623353																
4	85	0.0005	0.0005	0.3	0.3	0.25	0.25	0.45	0.45	0.13	0.4	2.00E-14	2.00E-14	1	100000	100000	1	222	12.3	100	36.5	0.0653119																
5	95	0.0005	0.0005	0.3	0.3	0.25	0.25	0.45	0.45	0.13	0.4	2.00E-14	2.00E-14	1	100000	100000	1	222	12.3	100	36.5	0.0572562																
6	105	0.0005	0.0005	0.3	0.3	0.25	0.25	0.45	0.45	0.13	0.4	2.00E-14	2.00E-14	1	100000	100000	1	222	12.3	100	36.5	0.0546369																
7	115	0.0005	0.0005	0.3	0.3	0.25	0.25	0.45	0.45	0.13	0.4	2.00E-14	2.00E-14	1	100000	100000	1	222	12.3	100	36.5	0.0627878																
8	125	0.0005	0.0005	0.3	0.3	0.25	0.25	0.45	0.45	0.13	0.4	2.00E-14	2.00E-14	1	100000	100000	1	222	12.3	100	36.5	0.0645318																
9	135	0.0005	0.0005	0.3	0.3	0.25	0.25	0.45	0.45	0.13	0.4	2.00E-14	2.00E-14	1	100000	100000	1	222	12.3	100	36.5	0.0238954																
10	145	0.00015	0.0005	0.3	0.3	0.25	0.25	0.45	0.45	0.13	0.4	2.00E-14	2.00E-14	1	100000	100000	1	222	12.3	100	36.5	0.0419281																
11	155	0.00025	0.0005	0.3	0.3	0.25	0.25	0.45	0.45	0.13	0.4	2.00E-14	2.00E-14	1	100000	100000	1	222	12.3	100	36.5	0.0320388																
12	165	0.00035	0.0005	0.3	0.3	0.25	0.25	0.45	0.45	0.13	0.4	2.00E-14	2.00E-14	1	100000	100000	1	222	12.3	100	36.5	0.0653119																
13	175	0.00045	0.0005	0.3	0.3	0.25	0.25	0.45	0.45	0.13	0.4	2.00E-14	2.00E-14	1	100000	100000	1	222	12.3	100	36.5	0.0618576																
14	185	0.00055	0.0005	0.3	0.3	0.25	0.25	0.45	0.45	0.13	0.4	2.00E-14	2.00E-14	1	100000	100000	1	222	12.3	100	36.5	0.0639764																
15	195	0.00065	0.0005	0.3	0.3	0.25	0.25	0.45	0.45	0.13	0.4	2.00E-14	2.00E-14	1	100000	100000	1	222	12.3	100	36.5	0.0651629																
16	205	0.00075	0.0005	0.3	0.3	0.25	0.25	0.45	0.45	0.13	0.4	2.00E-14	2.00E-14	1	100000	100000	1	222	12.3	100	36.5	0.0648332																
17	215	0.00085	0.0005	0.3	0.3	0.25	0.25	0.45	0.45	0.13	0.4	2.00E-14	2.00E-14	1	100000	100000	1	222	12.3	100	36.5	0.0642348																
18	225	0.00095	0.0005	0.3	0.3	0.25	0.25	0.45	0.45	0.13	0.4	2.00E-14	2.00E-14	1	100000	100000	1	222	12.3	100	36.5	0.0649383																
19	235	0.00105	0.0005	0.3	0.3	0.25	0.25	0.45	0.45	0.13	0.4	2.00E-14	2.00E-14	1	100000	100000	1	222	12.3	100	36.5	0.0655632																
20	245	0.00115	0.0005	0.3	0.3	0.25	0.25	0.45	0.45	0.13	0.4	2.00E-14	2.00E-14	1	100000	100000	1	222	12.3	100	36.5	0.0649434																
21	255	0.00125	0.0005	0.3	0.3	0.25	0.25	0.45	0.45	0.13	0.4	2.00E-14	2.00E-14	1	100000	100000	1	222	12.3	100	36.5	0.0645822																
22	265	0.00135	0.0005	0.3	0.3	0.25	0.25	0.45	0.45	0.13	0.4	2.00E-14	2.00E-14	1	100000	100000	1	222	12.3	100	36.5	0.0653668																
23	275	0.00145	0.0005	0.3	0.3	0.25	0.25	0.45	0.45	0.13	0.4	2.00E-14	2.00E-14	1	100000	100000	1	222	12.3	100	36.5	0.0649156																
24	285	0.00155	0.0005	0.3	0.3	0.25	0.25	0.45	0.45	0.13	0.4	2.00E-14	2.00E-14	1	100000	100000	1	222	12.3	100	36.5	0.0646544																
25	295	0.00165	0.0005	0.3	0.3	0.25	0.25	0.45	0.45	0.13	0.4	2.00E-14	2.00E-14	1	100000	100000	1	222	12.3	100	36.5	0.0656525																
26	305	0.00175	0.0005	0.3	0.3	0.25	0.25	0.45	0.45	0.13	0.4	2.00E-14	2.00E-14	1	100000	100000	1	222	12.3	100	36.5	0.0668902																
27	315	0.00185	0.0005	0.3	0.3	0.25	0.25	0.45	0.45	0.13	0.4	2.00E-14	2.00E-14	1	100000	100000	1	222	12.3	100	36.5	0.0646278																
28	325	0.00195	0.0005	0.3	0.3	0.25	0.25	0.45	0.45	0.13	0.4	2.00E-14	2.00E-14	1	100000	100000	1	222	12.3	100	36.5	0.0628583																
29	335	0.00205	0.0005	0.3	0.3	0.25	0.25	0.45	0.45	0.13	0.4	2.00E-14	2.00E-14	1	100000	100000	1	222	12.3	100	36.5	0.0613108																
30	345	0.00215	0.0005	0.3	0.3	0.25	0.25	0.45	0.45	0.13	0.4	2.00E-14	2.00E-14	1	100000	100000	1	222	12.3	100	36.5	0.0632233																
31	355	0.00225	0.0005	0.3	0.3	0.25	0.25	0.45	0.45	0.13	0.4	2.00E-14	2.00E-14	1	100000	100000	1	222	12.3	100	36.5	0.0645474																
32	365	0.00235	0.0005	0.3	0.3	0.25	0.25	0.45	0.45	0.13	0.4	2.00E-14	2.00E-14	1	100000	100000	1	222	12.3	100	36.5	0.0654471																
33	375	0.00245	0.0005	0.3	0.3	0.25	0.25	0.45	0.45	0.13	0.4	2.00E-14	2.00E-14	1	100000	100000	1	222	12.3	100	36.5	0.060741																
34	385	0.00255	0.0005	0.3	0.3	0.25	0.25	0.45	0.45	0.13	0.4	2.00E-14	2.00E-14	1	100000	100000	1	222	12.3	100	36.5	0.0649781																
35	395	0.00265	0.0005	0.3	0.3	0.25	0.25	0.45	0.45	0.13	0.4	2.00E-14	2.00E-14	1	100000	100000	1	222	12.3	100	36.5	0.0678578																
36	405	0.00275	0.0005	0.3	0.3	0.25	0.25	0.45	0.45	0.13	0.4	2.00E-14	2.00E-14	1	100000	100000	1	222	12.3	100	36.5	0.0687717																
37	415	0.00285	0.0005	0.3	0.3	0.1	0.25	0.6	0.45	0.13	0.4	2.00E-14	2.00E-14	1	100000	100000	1	222	12.3	100	36.5	0.0508117																
38	425	0.00295	0.0005	0.3	0.3	0.2	0.25	0.5	0.45	0.13	0.4	2.00E-14	2.00E-14	1	100000	100000	1	222	12.3	100	36.5	0.060737																
39	435	0.00305	0.0005	0.3	0.3	0.25	0.25	0.45	0.45	0.13	0.4	2.00E-14	2.00E-14	1	100000	100000	1	222	12.3	100	36.5	0.0645844																
40	445	0.00315	0.0005	0.3	0.3	0.4	0.25	0.3	0.45	0.13	0.4	2.00E-14	2.00E-14	1	100000	100000	1	222	12.3	100	36.5	0.0666825																
41	455	0.00325	0.0005	0.3	0.3	0.5	0.25	0.2	0.45	0.13	0.4	2.00E-14	2.00E-14	1	100000	100000	1	222	12.3	100	36.5	0.0678861																
42	465	0.00335	0.0005	0.3	0.3	0.6	0.25	0.1	0.45	0.13	0.4	2.00E-14	2.00E-14	1	100000	100000	1	222	12.3	100	36.5	0.0685344																
43	475	0.00345	0.0005	0.3	0.3	0.75	0.25	0.1	0.45	0.13	0.4	2.00E-14	2.00E-14	1	100000	100000	1	222	12.3	100	36.5	0.0672329																
44	485	0.00355	0.0005	0.2	0.3	0.35	0.25	0.45	0.45	0.13	0.4	2.00E-14	2.00E-14	1	100000	100000	1	222	12.3	100	36.5	0.0685976																
45	495	0.00365	0.0005	0.3	0.3	0.25	0.25	0.45	0.45	0.13	0.4	2.00E-14	2.00E-14	1	100000	100000	1	222	12.3	100	36.5	0.0630673																
46	505	0.00375	0.0005	0.4	0.3	0.15	0.25	0.45	0.45	0.13	0.4	2.00E-14	2.00E-14	1	100000	100000	1	222	12.3	100	36.5	0.0656909																
47	515	0.00385	0.0005	0.3	0.3	0.25	0.25	0.45	0.45	0.13	0.4	2.00E-14	2.00E-14	1	100000	100000	1	222	12.3	100	36.5	0.0631291																
48	525	0.00395	0.0005	0.1	0.3	0.25	0.25	0.65	0.45	0.13	0.4	2.00E-14	2.00E-14	1	100000	100000	1	222	12.3	100	36.5	0.0630717																
49	535	0.00405	0.0005	0.2	0.3	0.25	0.25	0.55	0.45	0.13	0.4	2.00E-14	2.00E-14	1	100000	100000	1	222	12.3	100	36.5	0.0631291																
50	545	0.00415	0.0005	0.3	0.3	0.25	0.25	0.45	0.45	0.13	0.4	2.00E-14	2.00E-14	1	100000	100000	1	222	12.3	100	36.5	0.0630673																
51	555	0.00425	0.0005	0.3	0.3	0.25	0.25	0.45	0.45	0.13	0.4	2.00E-14	2.00E-14	1	100000	100000	1	222	12.3	100	36.5	0.0630673																
52	565	0.00435	0.0005	0.5	0.3	0.25	0.25	0.25	0.45	0.13	0.4	2.00E-14	2.00E-14	1	100000	100000	1	222	12.3	100	36.5	0.0631303																
53	575	0.00445	0.0005	0.6	0.3	0.25	0.25	0.15	0.45	0.13	0.4	2.00E-14	2.00E-14	1	100000	100000	1	222	12.3	100	36.5	0.063068																
54	585	0.00455	0.0005	0.7	0.3	0.25	0.25	0.05	0.45	0.13	0.4	2.00E-14	2.00E-14	1	100000	100000	1																					

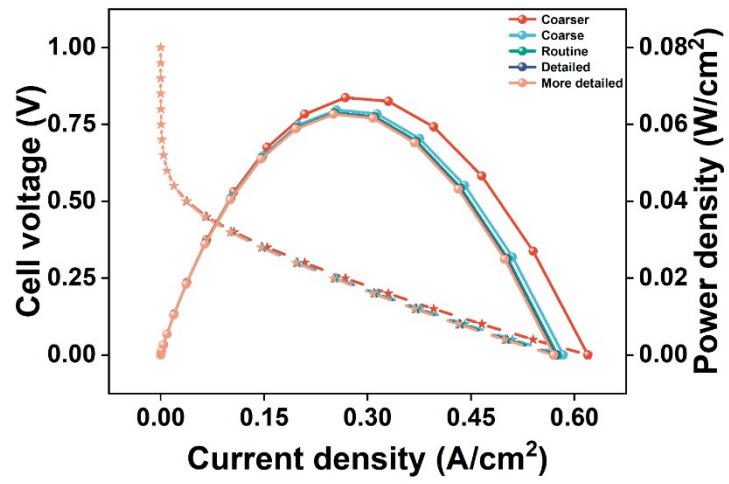


Figure S1. DMFC Grid Consistency Verification.

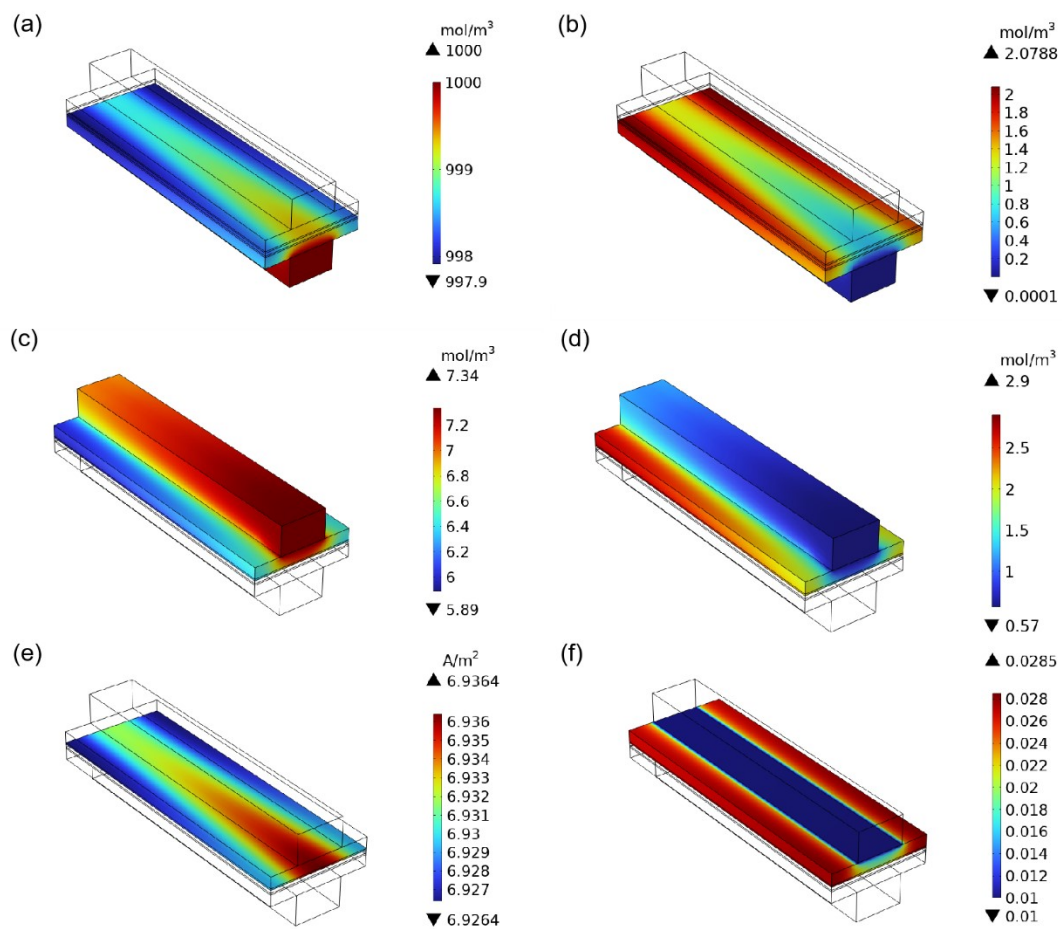


Figure S2. Concentration distribution of reactants and products (0.25 V): (a) Molar concentration of methanol at the anode, (b) Molar concentration of CO_2 at the anode, (c) Molar concentration of oxygen at the cathode, (d) Molar concentration of water at the cathode. Cross current density generated by methanol infiltration at the anode (0.25 V). Liquid Saturation at Cathode GDL and CL (0.25 V).

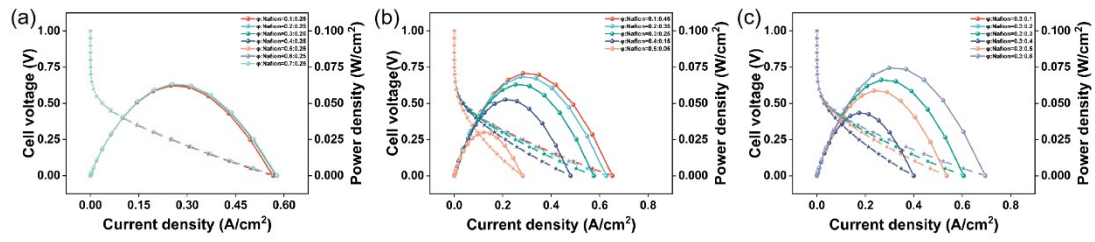


Figure S3. Polarization curve obtained by changing the ratio between porosity and nafion in the catalyst layer; (a) Porosity changes, nafion remains unchanged; (b) Porosity changes, nafion changes; (c) Porosity remains unchanged and nafion changes.

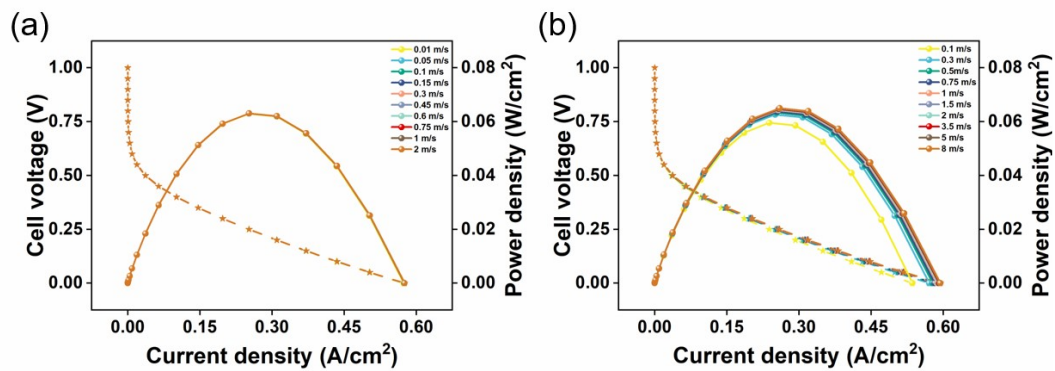


Figure S4. Polarization curve obtained by changing the inlet velocity of methanol at the anode and oxygen at the cathode.

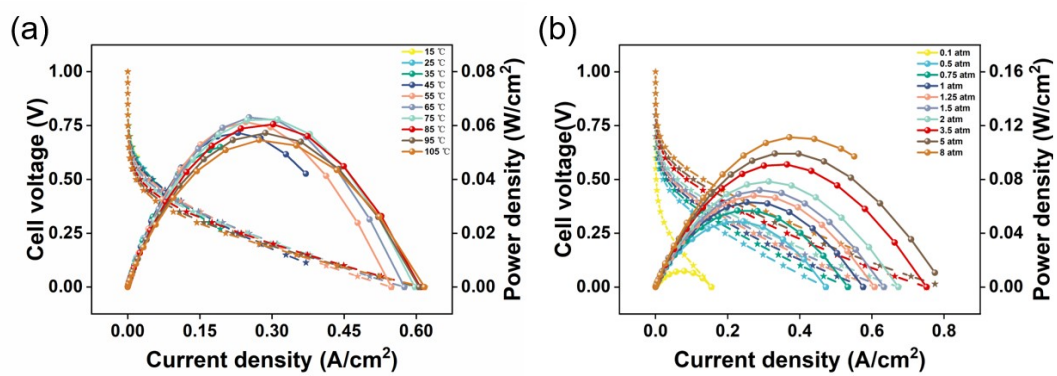


Figure S5. Polarization curve obtained by changing temperature and pressure.

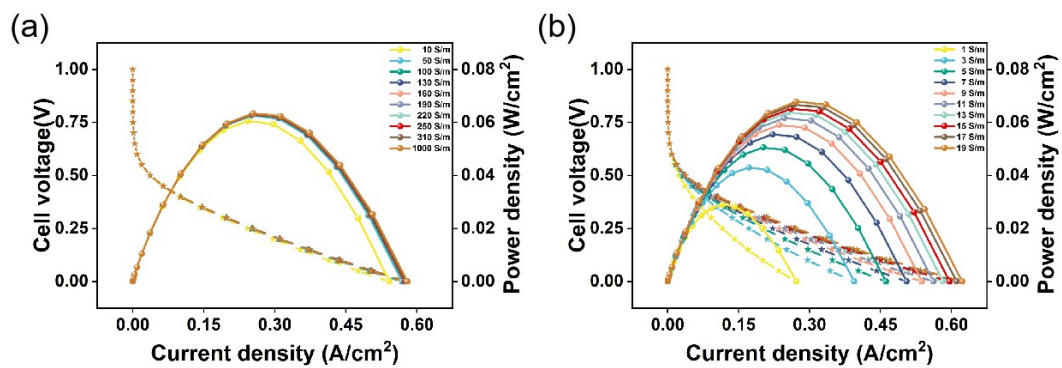


Figure S6. Polarization curves obtained by changing (a) electron conductivity and (b) proton conductivity.

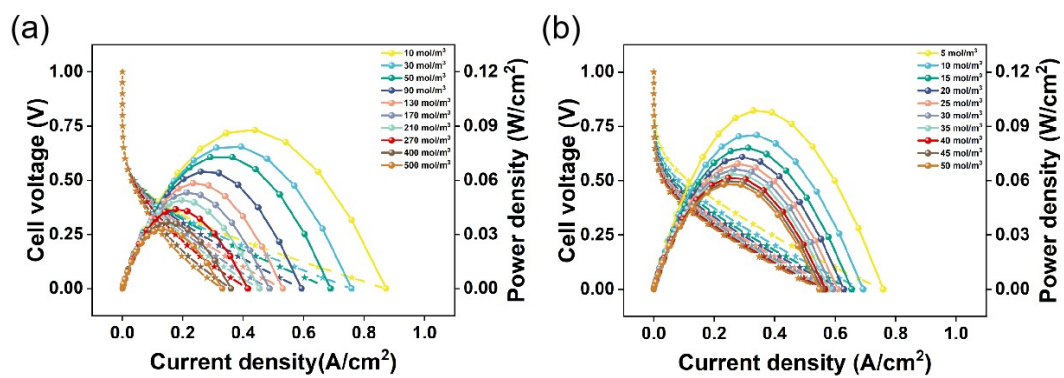


Figure S7. Polarization curve obtained by changing (a) anode methanol concentration and (b) cathode oxygen concentration.

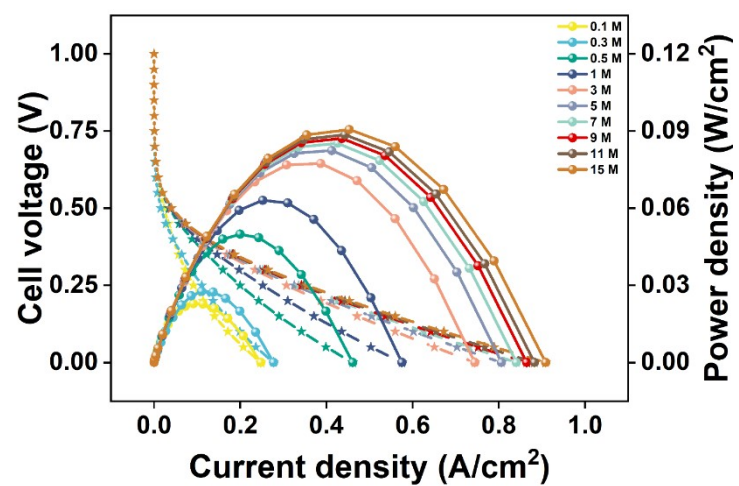


Figure S8. Polarization curve obtained by changing anode methanol inlet concentration.

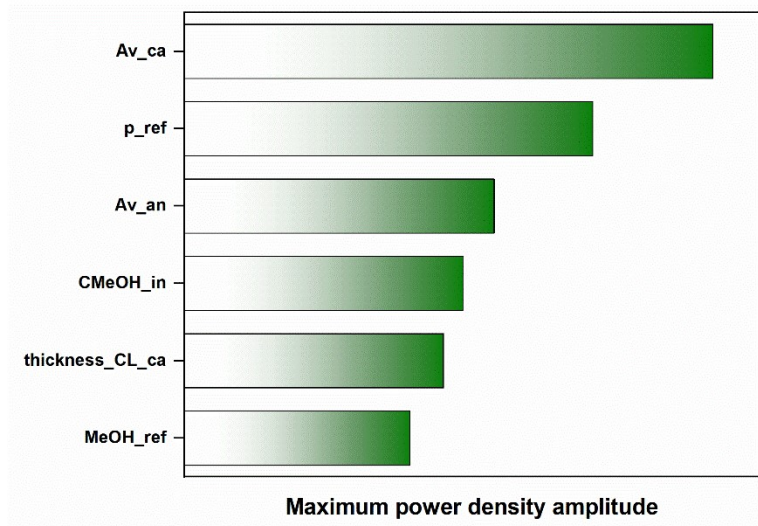


Figure S9. The influence of different parameters on the maximum power density amplitude of fuel cells from simulation model (top 6).

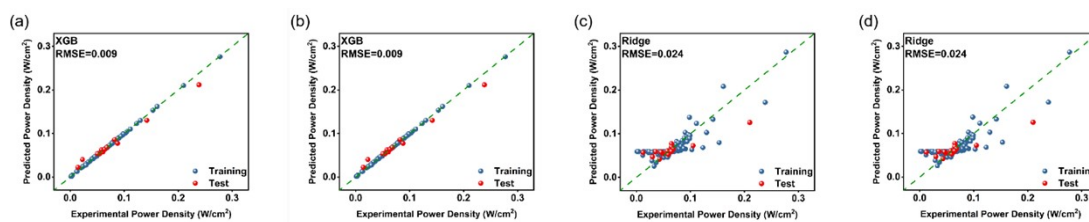


Figure S10. The other four algorithms' data training test (90% - 10%) error plots. (a)KRR; (b)LASSO; (c)RIDGE; (d)SVR. Training data (blue), test data (red).

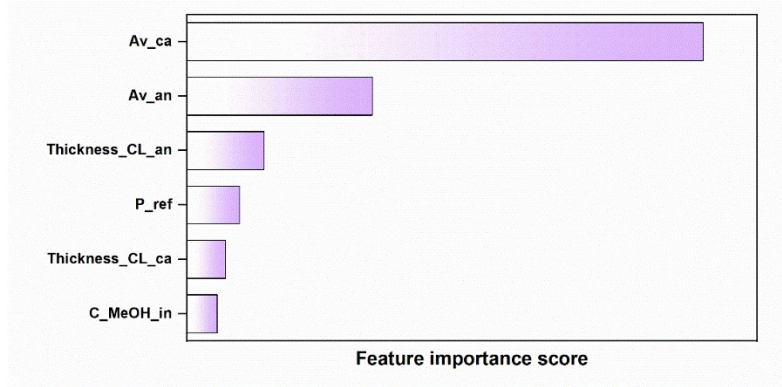


Figure S11. Average feature importance prediction plots using the ratio of maximum power density to different pressures based on the best ETR models in ten-fold cross-validation (top 6).