

SUPPLEMENTARY MATERIALS

Table S1 Experimental data in the processes of kiln, NH₃, urea, MeOH

Kiln					
Composition			Vol%		
CO ₂			18.9		
N ₂			60.6		
H ₂ O			12.8		
O ₂			7.7		
Ammonia synthesis reaction					
Pressure (atm)			Mole fraction of ammonia		
11.90476			0.517301		
29.10053			0.632353		
50.26455			0.759516		
100.5291			0.810554		
201.0582			0.878893		
400.7937			0.911765		
1001.323			0.964533		
Urea synthesis reaction					
Ratio of NH ₃ /CO ₂			Mole fraction of urea		
1.942141			0.639897		
2.517574			0.688657		
2.990019			0.720177		
3.498908			0.770122		
4.004426			0.79986		
4.542522			0.824844		
5.509972			0.8231		
7.551729			0.86003		
9.525555			0.889826		
11.49789			0.910707		
19.54686			0.950847		
Methanol synthesis reaction					
10 bar		30 bar		60 bar	
Temperature (°C)	CO ₂ Conversion	Temperature (°C)	CO ₂ Conversion	Temperature (°C)	CO ₂ Conversion
100.6378	0.398769	99.36224	0.738949	101.2755	0.923694
149.7449	0.227071	149.7449	0.439681	149.7449	0.738801
200.7653	0.16827	200.7653	0.298769	200.1276	0.460061
250.5102	0.16959	248.5969	0.248775	249.2347	0.327952
300.2551	0.216365	300.2551	0.23836	350.6378	0.311526

350	0.274871	349.3622	0.299799	300.8929	0.288211
399.7449	0.35537	399.7449	0.3671	399.7449	0.397892
450.1276	0.428536	449.4898	0.450532	450.1276	0.481322
499.8724	0.511968	499.8724	0.517833	499.8724	0.519299
550.2551	0.548477	550.2551	0.549943	550.2551	0.548477
599.3622	0.571793	599.3622	0.579125	599.3622	0.580591

Table S2 Mathematical models of PEM water electrolysis

Voltage	$V(T, p) = e_{rev}(T, p) - e_{rev}(T, p)e^{\frac{-5I}{0.02}} + IR_i(T, p)$
Current	$I(T, p) = 0 \quad V \leq e_{rev}(T, p)$ $I(T, p) = \frac{1}{R_i(T, p)}(V - e_{rev}(T, p)) \quad V \geq e_{rev}(T, p)$
Initial resistance of PEM system	$R_i(T, p) = R_{i0} + k \ln\left(\frac{p}{p_0}\right) + dR_t(T - T_0)$
Reverse voltage	$e_{rev}(T, p) = e_{rev,0} + \frac{R(273 + T)}{2F} \ln\left(\frac{p}{p_0}\right)$
The ideal voltage	$V_i = \frac{\Delta G}{2F}$
Gibbs free energy change of H ₂	$\Delta G = 285.84 - 163.2(273 + T)$
Hydrogen production rate	$v_H = \frac{60000v_m I}{2F}$
Molar volume rate (Ideal Gas)	$v_m = \frac{R(273 + T)}{p}$
Input power	$P = I^2 R_i + I e_{rev} = R_i \left(\frac{2Fv_H}{60000v_m} \right)^2 + \left(\frac{2Fv_H}{60000v_m} \right) e_{rev}$

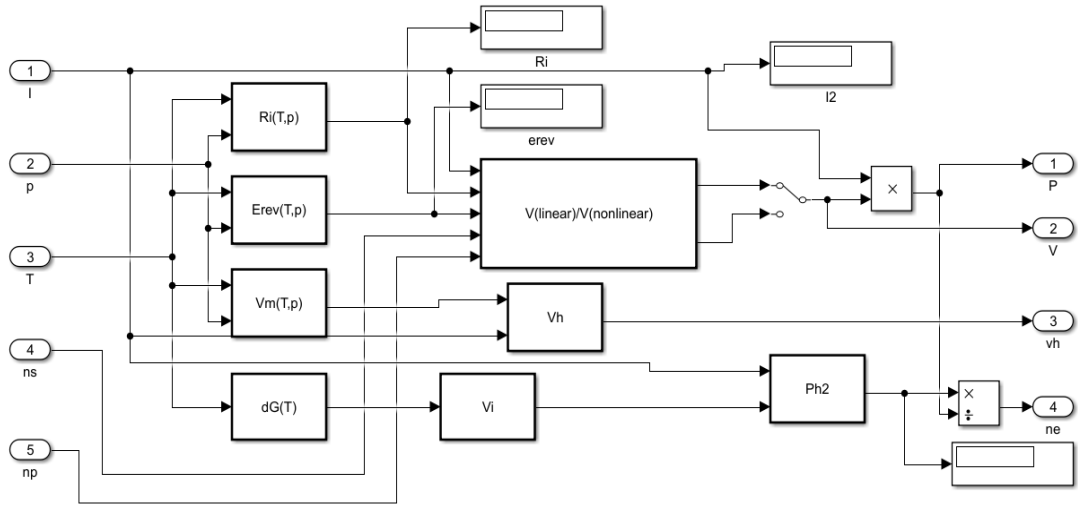


Figure S1 Flowchart of PEM water electrolysis with Simulink™