

Supporting Information

Electrochemical Ammonia Compression

Ye Tao,^a William Gibbons,^a Yunho Hwang,^b Reinhard Radermacher,^b Chunsheng Wang^{*a}

^a Department of Chemical and Biomolecular Engineering, University of Maryland, College Park, MD 20742, USA

^b Center for Environmental Energy Engineering, University of Maryland, College Park, MD 20742, USA

*Corresponding Author: Chunsheng Wang (cswang@umd.edu)

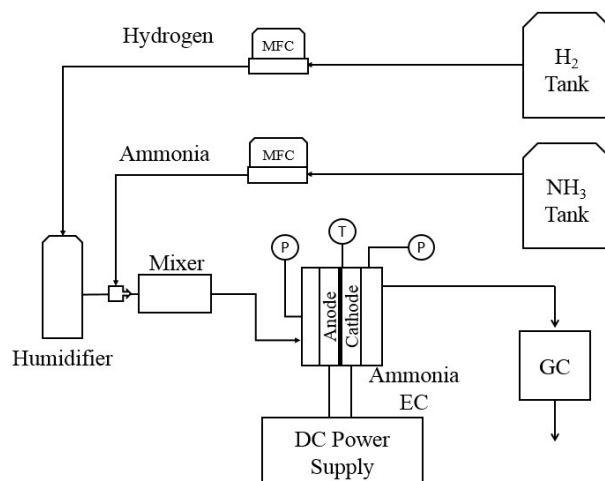


Figure S1: The schematic of electrochemical NH₃ compression testing facility for in-situ GC measurement

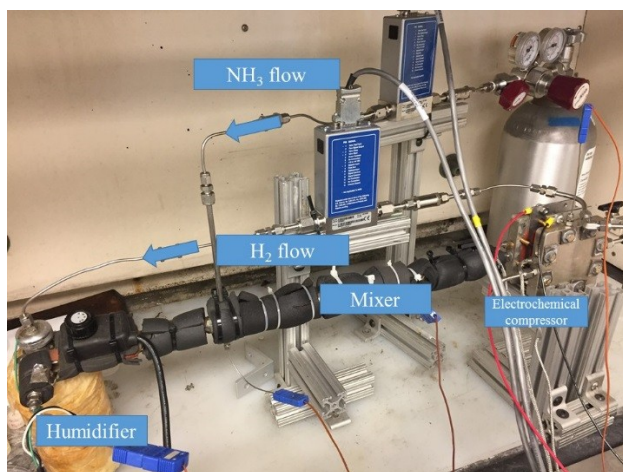


Figure S2: Picture of electrochemical ammonia compression testing facility

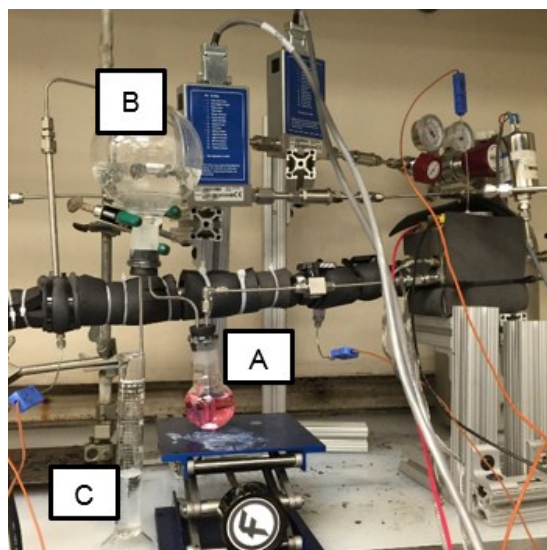


Figure S3: The titration system built for continuous quantitative analysis of NH_3 and H_2

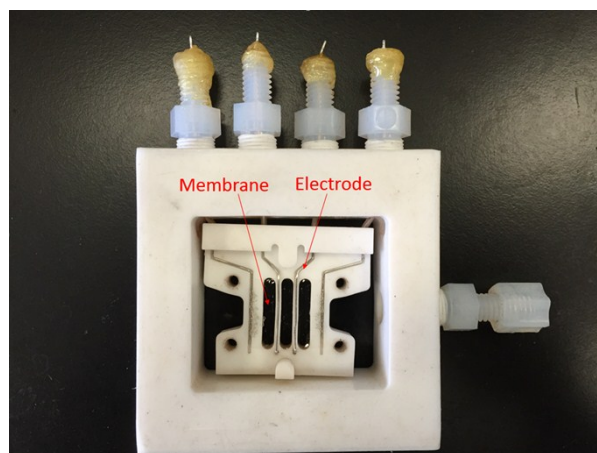


Figure S4: The membrane placed in between electrodes in BekkTech BT-112 for NH_4^+ conductivity measurement

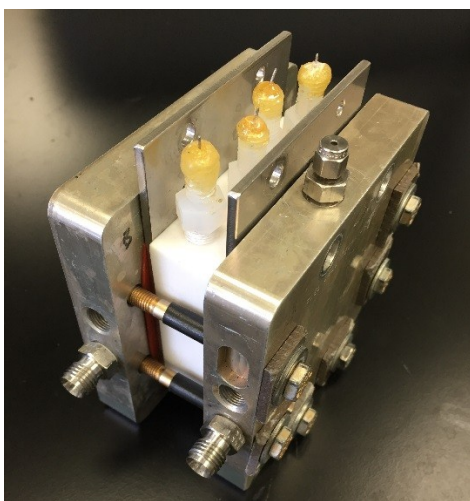


Figure S5: The BakkTech BT-112 module is sandwiched in between original electrochemical compression device, the same device shown in Figure S2 and S3

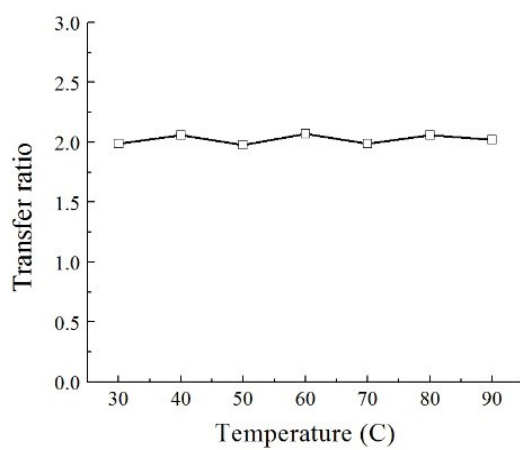


Figure S6: NH₃/H₂ transfer ratio vs. temperature

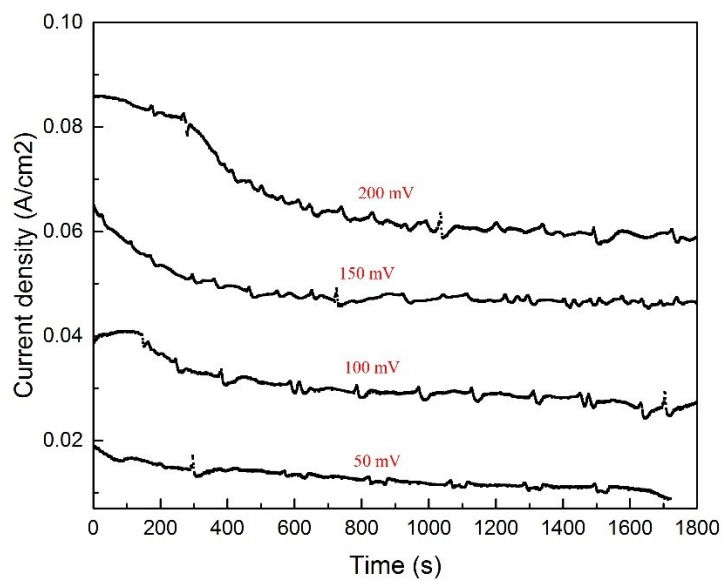


Figure S7: Current density vs time at constant voltage charge (50mV, 100mV, 150mV, 200mV) with cathode back pressure, current density decreases due to cathode pressure built up and eventually stabilizes

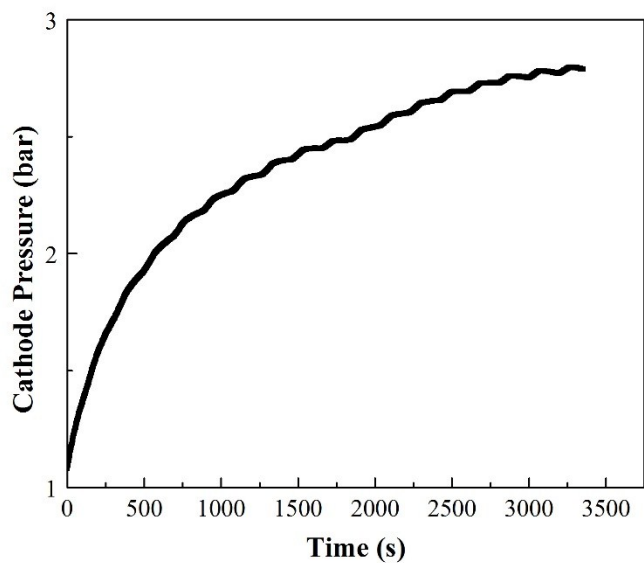


Figure S8: Cathode pressure vs. time at constant voltage of 50 mV

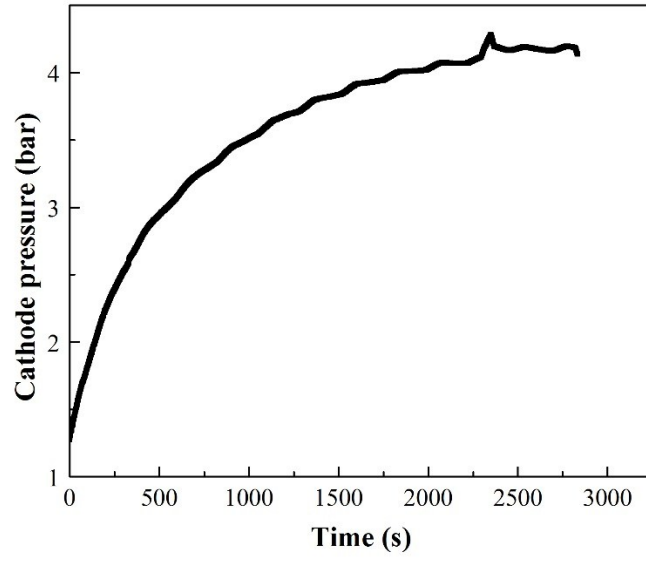


Figure S9: Cathode pressure vs. time at constant voltage of 100 mV

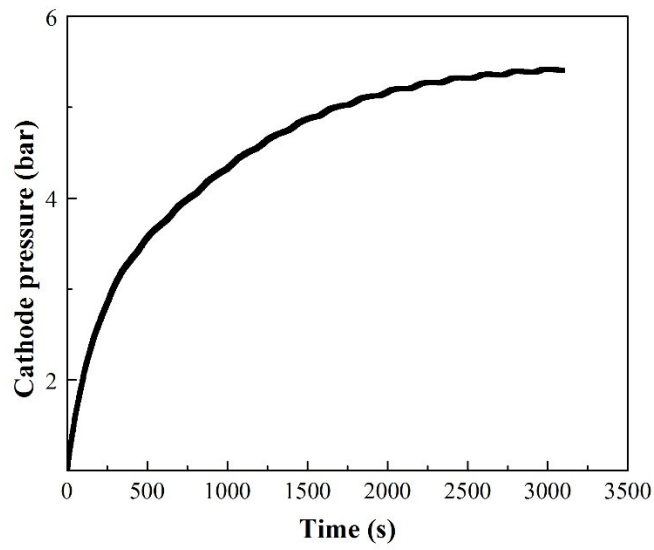


Figure S10: Cathode pressure vs. time at constant voltage of 150 mV

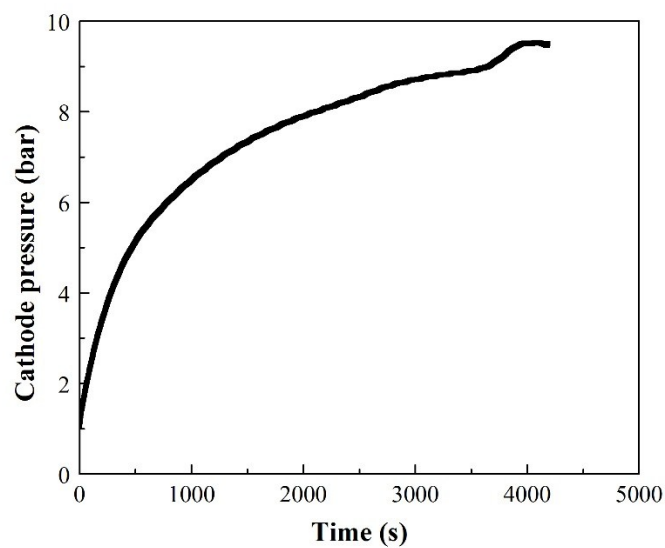


Figure S11: Cathode pressure vs. time at constant voltage of 200 mV

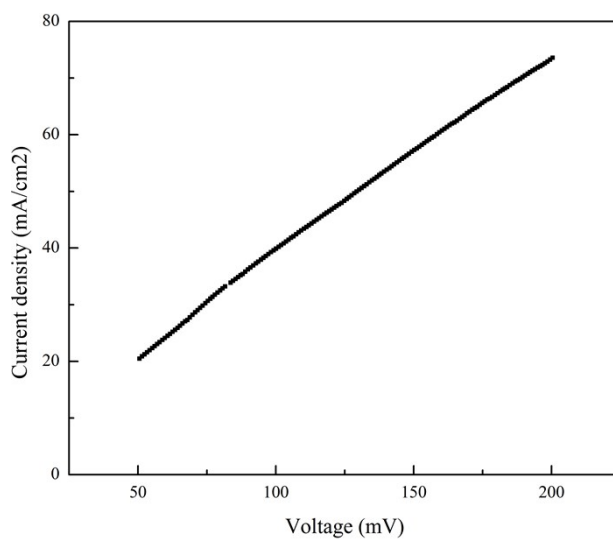


Figure S12: Measured current density vs. voltage in a linear sweep at 0.5 mV/s from 50 mV to 200 mV at 50% RH (H₂ and NH₃ supplied to anode)

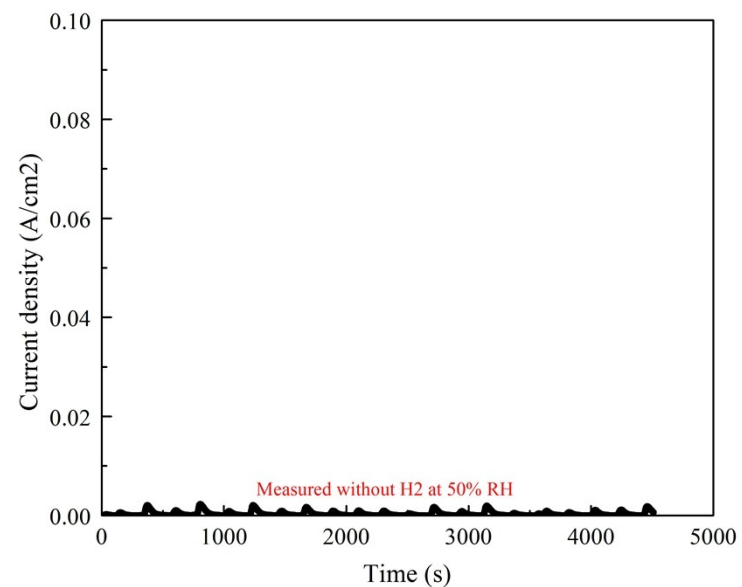


Figure S13: Current density of NH₃ flow at constant voltage 200 mV measured over time without H₂ fed to the anode (humidified NH₃ supplied to anode)

Table S1 – Feed composition in the inlet and measured composition in outlet (cathode) using titration method

Inlet feed ratio	Measured gas molar ratio in outlet (NH ₃ /H ₂)
4.0	2.55
2.5	2.17
2.0	2.06

Table S2: Ammonia composition adjusted based on crossover amount due to concentration gradient

Feed Ratio	H ₂ peak area (V*sec)	H ₂ concentration	Original NH ₃ peak area(V*sec)	Original NH ₃ concentration	NH ₃ crossover peak area(V*sec)	NH ₃ peak area adjusted(V*sec)	NH ₃ concentration adjusted	Original Gas composition ratio	Gas composition ratio adjusted
4:1	0.50	0.29	0.43	0.67	0.05	0.38	0.59	2.30	2.03
2.5:1	0.52	0.31	0.42	0.66	0.03	0.39	0.61	2.16	2.00

The adjusted gas ratio in the final column was the measured value after correcting for crossover of NH₃. For measuring the cross over amount, both anode and cathode pressure were maintained at around 1 atm.

Table S3: Comparison between titration measured flowrate and theoretical

Feed NH ₃ /H ₂ (sccm)	Theoretical H ₂ (mol/s)	Theoretical NH ₃ (mol/s)	Titration measured H ₂ (mol/s)	Titration measured NH ₃ (mol/s)
100/50	7.25e-07	1.45e-06	8.77±0.61e-07	1.89±0.13e-06
100/50	7.25e-07	1.45e-06	8.62±0.60e-07	1.86±0.13e-06
100/50	7.25e-07	1.45e-06	8.90±0.62e-07	1.94±0.14e-06

The compression efficiency calculation:

The compression efficiency in a continuous compression system is defined in Equation S1 as the ratio between power of compression and power input. The isothermal compression work is calculated based on Equation S2, which is equal to the Nernst potential multiplied by the current. The real work input is calculated in Equation S3. Therefore the compression efficiency can be derived in Equation S4. The isothermal compression process of EC achieved by thermal management similarly implemented in PEMFC has less irreversible loss than isentropic mechanical compressor.

$$\eta_c = \frac{W_{compression}}{W_{input}} \quad (S1)$$

$$W_{compression} = \frac{RT_{EC}}{nF} \ln \left(\left(\frac{P_{H2, outlet}}{P_{H2, inlet}} \right)^{\frac{1}{2}} * \left(\frac{P_{NH3, outlet}}{P_{NH3, inlet}} \right) \right) \times I \quad (S2)$$

$$W_{input} = U_{cell} \times I \quad (S3)$$

$$\eta_c = \frac{W_{compression}}{W_{input}} = \frac{\frac{RT_{EC}}{nF} \ln \left(\left(\frac{P_{H2, outlet}}{P_{H2, inlet}} \right)^{\frac{1}{2}} * \left(\frac{P_{NH3, outlet}}{P_{NH3, inlet}} \right) \right)}{U_{cell}} \quad (S4)$$

At 50 mV of voltage supply and anode pressure around 1 bar, the cathode pressure is measured to be 2.8 bar in a continuous compression flow, and the compression ratio is 2.8, which satisfies the compression ratio required by the mechanical compressor in the ammonia vapor compression system, and the Nernst voltage is calculated by equation 6 to be 47 mV. Therefore, the electrochemical compression efficiency is 93% based on equation 10, which is much higher than 65% given by the mechanical compressor.