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Office of ENERGY EFFICIENCY & RENEWABLE ENERGY

AMMTO & IEDO JOINT PEER REVIEW

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Washington, D.C.

Compact Catalytic Membrane Reactor for One-Step High-Efficiency Ammonia (NH_3) Synthesis at Moderate Temperatures and Pressures | IEDO

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Contract Number: DE-EE0009409 **|** Project Period: May 2021 – April 2024

This presentation does not contain any proprietary, confidential, or otherwise restricted information

Project Overview

This work supports IEDO's mission to accelerate innovations for energy and emission reductions with through the following impacts:

- ✓ Global production capacity of NH_3: ~235 million metric tons in 2019, expected to nearly 290 million metric tons by 2030.
- ✓ Ammonia production consumes ~2% of the world's energy and generates 1% of global CO_2 emission.
- ✓ Over 90% of NH_3 is synthesized by the energy-intensive Haber-Bosch (HB) process at 200-300 bar and 450-550 ℃.
- ✓ Step-out reductions of unit operations from process intensification with our innovative catalytic membrane reactor NH_3 synthesis technology integrated reaction/separation
- ✓ Significantly lower energy intensity and flexible to variable operating inputs.
- ✓ A very compact modular system and small footprint at desired small or large scales.

Energy, Emissions, & Environment: Reduce >80% energy consumption	**Cost & Competitiveness:** Reduce > 80% operating cost
Technical & Scientific: >50 % N_2 conversion in single-pass	**Other Impacts:** Compact modular design and flexible scales

Project Outline

Innovation: Revolutionary process and a unique compact catalytic membrane reactor with integrated reaction and separation, along with a high packing-density hollow fiber membrane reactor configuration, enables a compact modular system for energy and cost-efficient NH_3 synthesis at desired scales

Project Lead: E2H2NANO, LLC

Project Partners: University at Buffalo, University of South Carolina

Timeline: April 1, 2021- April 30, 2024, 60% completed

Budget: $2,435,928 (DOE: $1,945,854, Cost share:$ 490,074)

	FY21 Costs	FY22 Costs	FY23 Costs	Total Planned Funding
DOE Funded	$184,570	$674,634	$1,086,650	$1,945,854
Project Cost Share	$54,110	$223,871	$212,093	$490,074

End Project Goal: Achieve >50% single-pass N_2 conversion, 80-90% energy consumption reduction, >80% operating cost reduction, and <10% performance degradation of catalytic membrane reactor in 120 h.

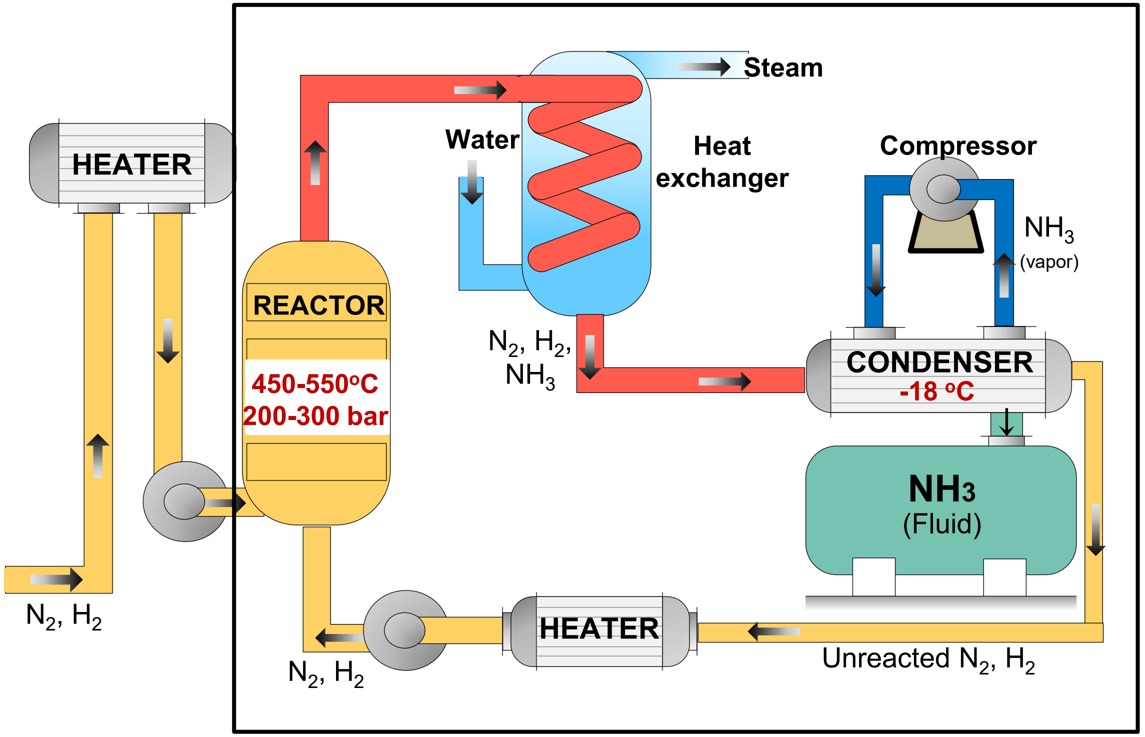
Background & Strategic Approach

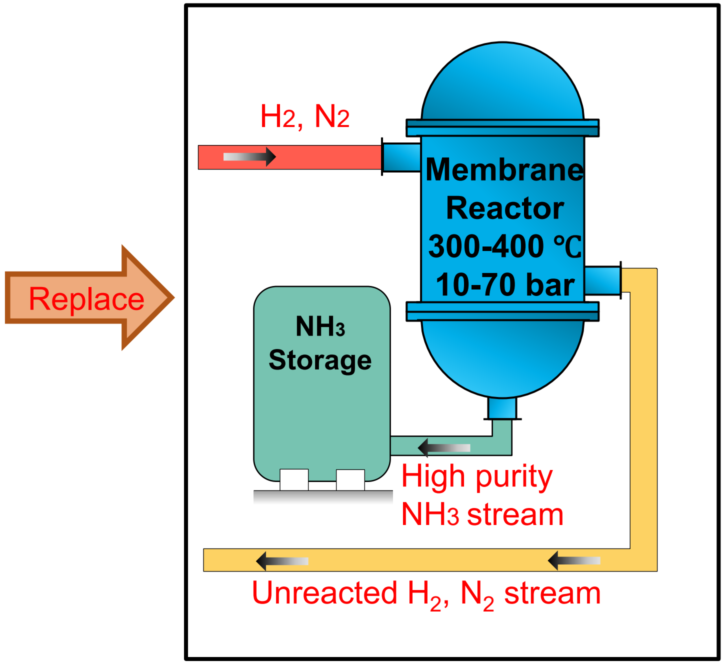
Commercial NH_3 production via HB process:

- Extreme operating conditions: 450-550 °C, 200-300 bar
- Low N_2 conversion (~15% single pass), large quantity of unreacted gas mixture recycling and reheating
- Cryogenic condensation (-18 – -24 °C) for NH_3 recovery
- High cost and massive energy consumption

Our proposed technology:

- Compact membrane reactor
- Mild operating conditions: 300-400 °C, 10-70 bar
- High N_2 conversion (>50% single pass)
- Eliminated cryogenic condensation for NH_3 recovery
- Low cost and energy efficient process





Reference: Modified based on https://en.wikipedia.org/wiki/Haber_process

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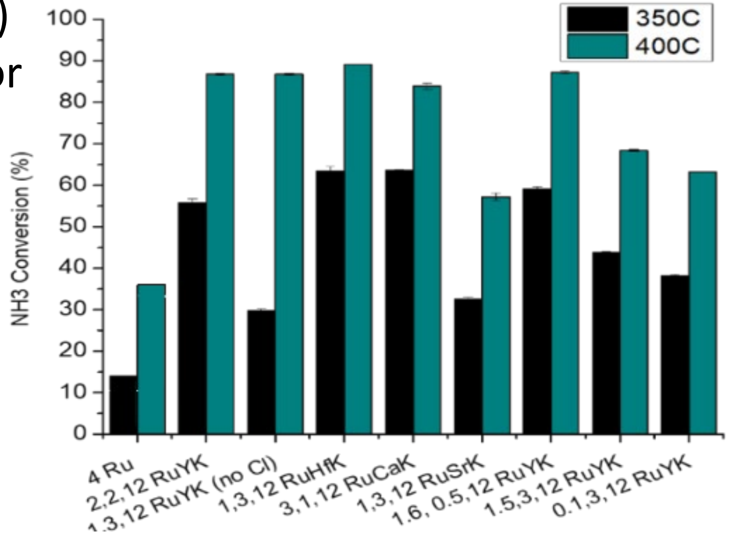
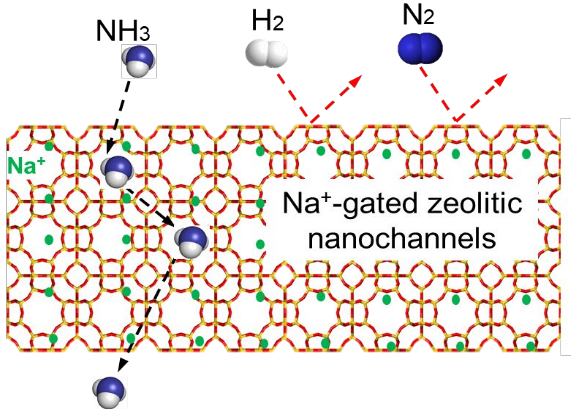
Two key components: Ru-based catalyst and Na^+-gated, nanochannel membrane

Artificial Intelligence (AI) assisted development for nano-engineered, low-cost Ru-based catalyst: High activity for NH_3 decomposition and synthesis at moderate reaction temperatures and pressures.



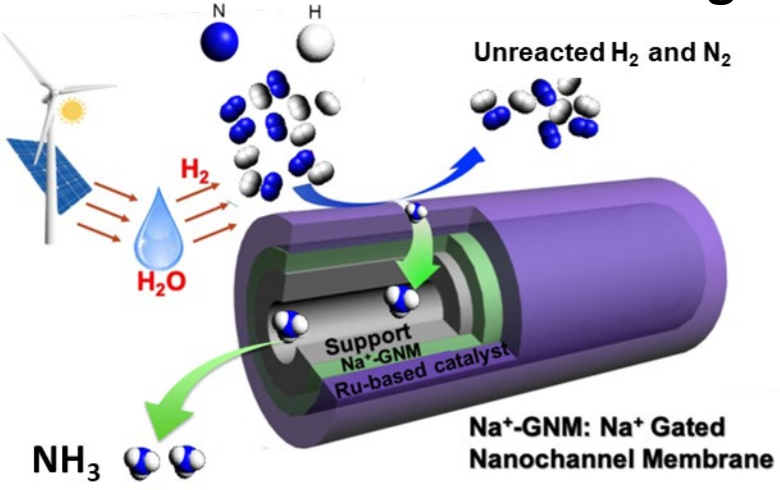
Science AAAS Vol 367 (6478), 667-671, 2020

WATER AND AMMONIA HAVE SIMILAR SIZE AND POLARITY!



Our unique Na^+-gated, nanochannel membrane only allows fast transport of small, polar molecules (such as H_2O and NH_3), whereas blocks the permeation of larger molecules.

Proposed membrane reactor integrated reaction and separation



Catalytic membrane reactor has hollow fibers with Na^+-gated nanochannel membrane to separate NH_3 from N_2 and H_2 in situ, shifting the thermodynamic equilibrium towards continuous NH_3 formation with higher single-pass conversion rates.

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Risks:

- ✓ Catalyst deactivation
- ✓ Membrane performance not in the desired range
- ✓ NH_3 yield not sufficiently high

Mitigation strategies:

- ✓ Add promotors to improve catalyst poisoning resistance
- ✓ Adjust reaction temperature or catalyst regeneration
- ✓ Improve membrane synthesis
- ✓ Optimize MR design, optimize operation conditions

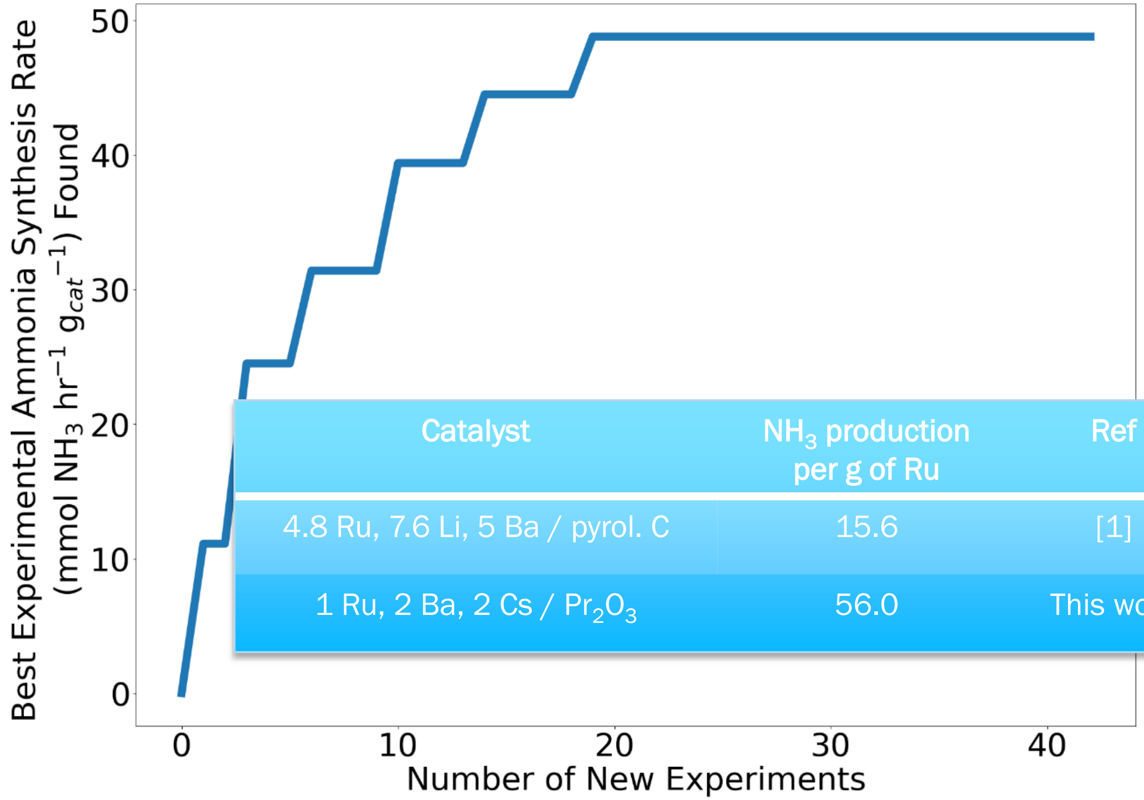
Team:

Member	Roles
E2H2NANO	• Lead on project management and planning, and market transformation • Lead on membrane reactor design, construction, and testing • Support membrane and catalyst development
University of South Carolina	• Lead on catalyst synthesis and QA/QC testing • Support membrane reactor design, construction, and testing
UB	• Lead on membrane and module fabrication and QA/QC testing • Support membrane reactor design, construction, and testing

Results and Achievements

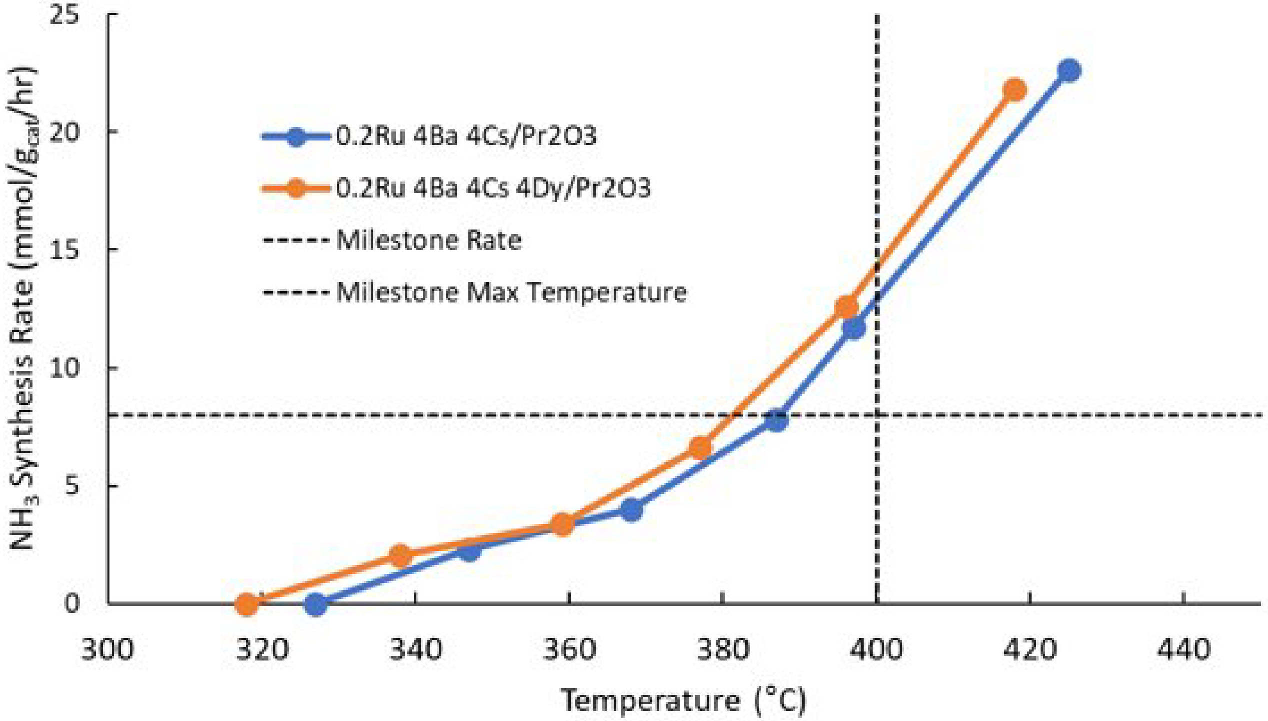
Highly active, low-cost Ru-based catalyst developed with Artificial Intelligence (AI)

- Machine learning (ML) allows for rapid discovery of novel catalyst formulations



Catalyst	NH_3 production per g of Ru	Ref
4.8 Ru, 7.6 Li, 5 Ba / pyrol. C	15.6	[1]
1 Ru, 2 Ba, 2 Cs / Pr_2O_3	56.0	This work

- Performance of <0.2 wt.% Ru-based catalyst with Promoters meet the milestones

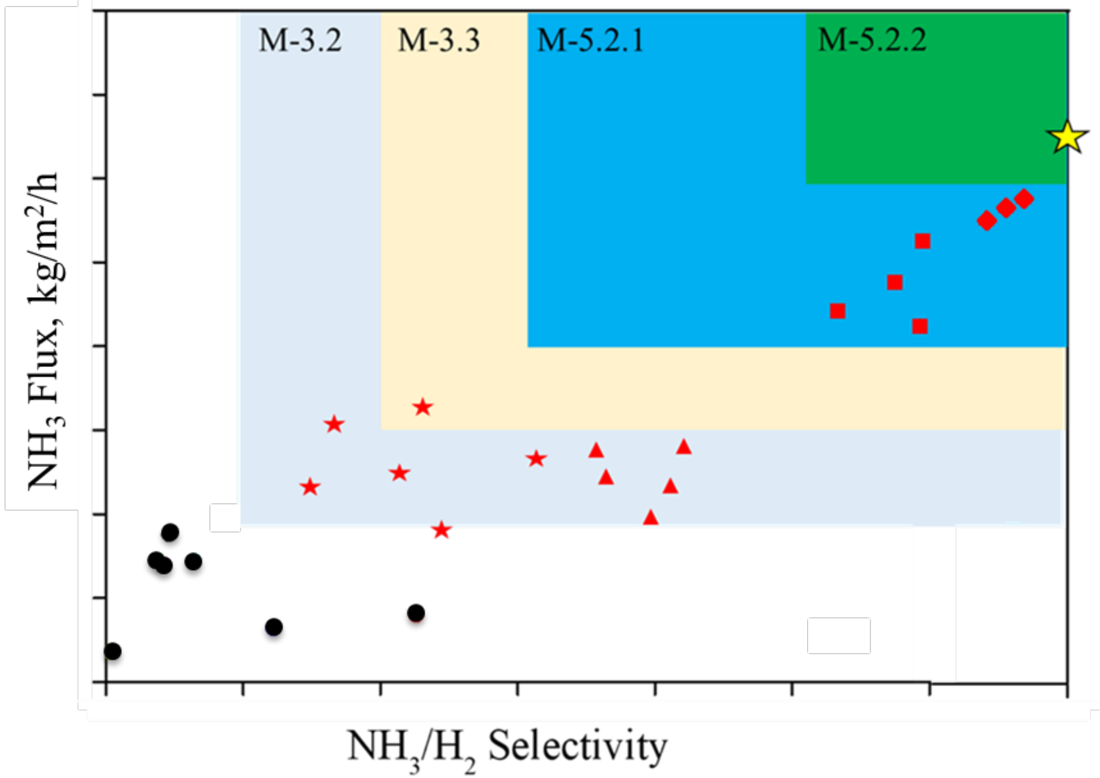


1. Zheng, J; et al. *Angew. Chem.* (2019), 58, 48.

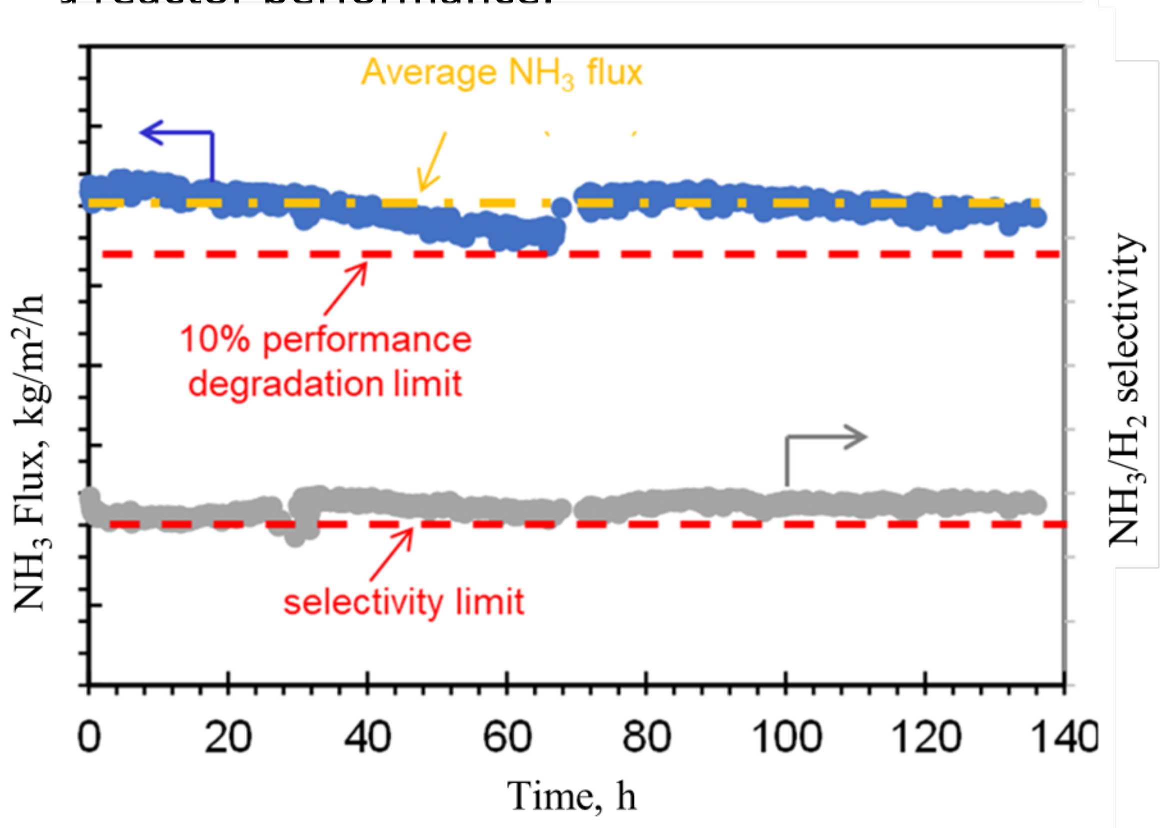
Results and Achievements pg. 2

Highly NH_3 selective Na^+- gated nanochannel membrane development

- All membrane development milestones have been met, allowing for efficient, low-energy separation with sufficient NH_3 flux and selectivity for targeted reactor performance.



Black symbols indicate initial membrane performances
Red symbols represent membrane performances achieved at the different stages during the project
Yellow star is the highest membrane performance achieved



*Note: NH_3/N_2 selectivity of >1,000

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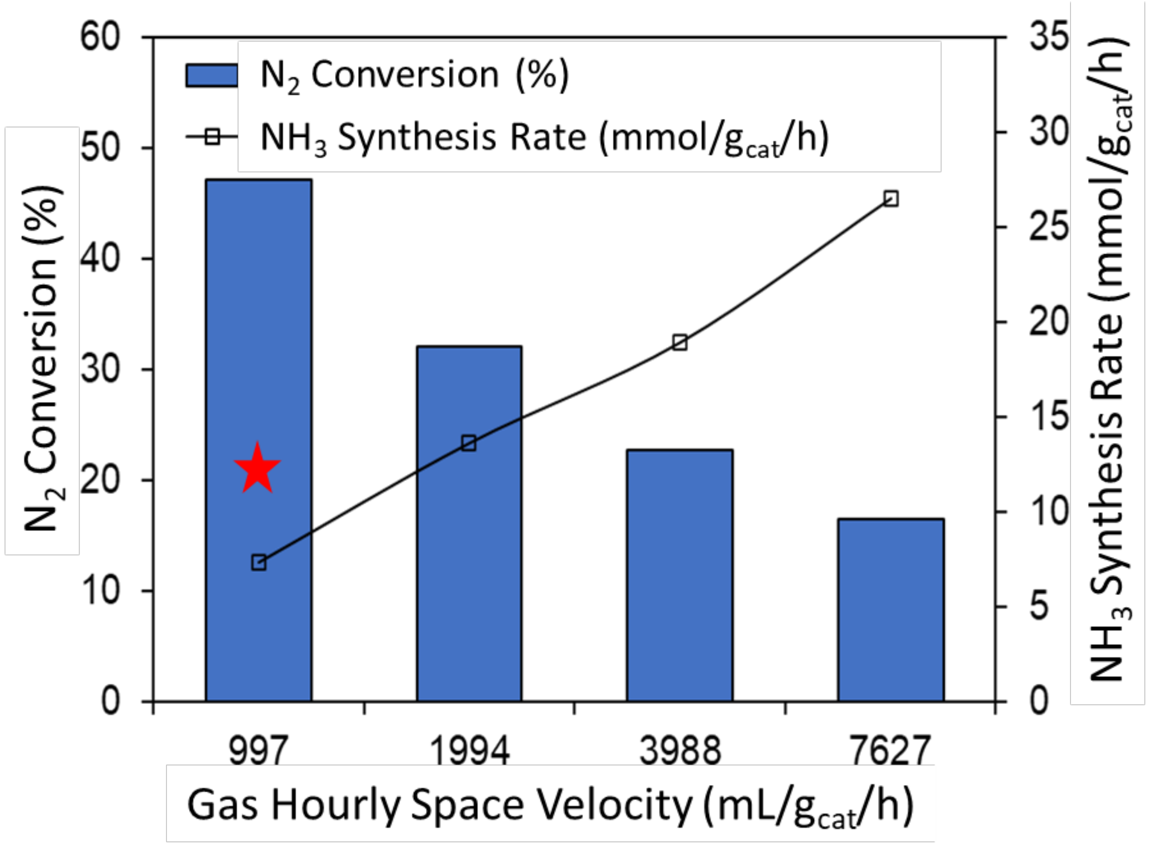
N_2 conversion for NH_3 synthesis in lab-scale membrane reactor doubled the equilibrium conversion



- Maximum conversion achieved 47.27% vs equilibrium 23.25% (★)
- Our technology saves 53.8% energy requirement
- Our technology saves 65% operating cost

Patents and publications:

Provisional patent, Ion-gated nanochannel catalytic membrane reactor.

S Padinjarekutt et al., Synthesis of Na^+-gated nanochannel membranes for the ammonia (NH_3) separation. Journal of Membrane Science, 674, 121512.

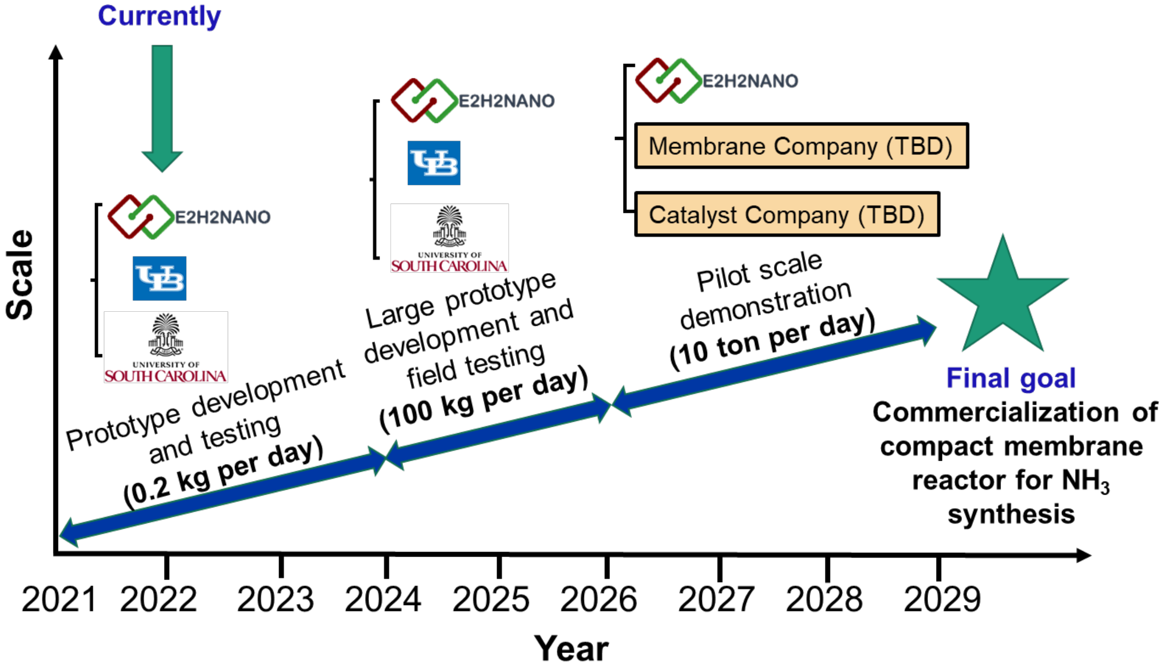
Future Work, Technology Transfer, & Impact

Future Work:

- ✓ Demonstrate a 0.2kg/day production of NH_3 production using a membrane reactor

Technology Transfer:

- ✓ De-risk the scaling of our technology and collect performance and cost data;
- ✓ Demonstrate the value proposition of our technology for NH_3 synthesis to our potential customers;
- ✓ Use renewable energy industry or industry with H_2 byproduct as a test bed for early adoption of our technology;
- ✓ Develop models, tools, and templates for customers to provide best practices in real-world implementation.



Impacts:

- ✓ Our innovative approach incorporating reaction and separation overcomes thermodynamic and kinetic barriers and achieves high N_2 conversion and NH_3 yield at moderate temperatures and pressures.
- ✓ Our technology is less energy-intensive (>80% improvement) and more economical, making it a promising solution for decarbonizing energy and emission intensive industries.
- ✓ Our technology is expected to have a flexible equipment size with small footprint modular design, making it easier to integrate into the existing systems.

Questions?

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