Ammonia Use in Medium/Heavy-Duty Internal Combustion Applications

Cosmin Dumitrescu
Mechanical, Materials, and Aerospace Engineering
West Virginia University

NETL Ammonia Combustion Technical Working Group Meeting

November 12, 2024

West Virginia University
CENTER FOR ALTERNATIVE FUELS ENGINES AND EMISSIONS

Advanced Combustion

PCFI LABORATORY

West Virginia University
CENTER FOR INNOVATION IN GAS RESEARCH AND UTILIZATION

Why Use Ammonia (NH_3) for Power Generation

Carbon-Free Combustion: NH_3 combustion produces nitrogen (N_2) and water (H_2O), and no carbon dioxide (CO_2) emissions. Hence, a viable option for decarbonizing power generation.

High Energy Density: NH_3 has a relatively high energy density compared to some other alternative fuels, making it efficient for storage and transport.

Existing Infrastructure: NH_3 is already widely used in the chemical and fertilizer industries, with established global production, storage, and transport infrastructure that can be adapted for energy use.

Why Use Ammonia (NH_3) for Power Generation

Versatile Production Pathways: NH_3 from green hydrogen (H_2; via electrolysis powered by renewable energy) and N_2 from the air, enabling a fully renewable and sustainable energy cycle.

Potential for Co-Firing: NH_3 can be co-fired with other fuels (natural gas, coal) in existing power plants. Hence, NH_3 provides a transitional step toward decarbonization that doesn’t require an entirely new infrastructure.

Global Energy Carrier: NH_3 easier to liquefy and store compared to H_2, which reduces logistical challenges. Therefore, NH_3 can serve as an energy carrier for H_2, facilitating long-distance energy trade.

Challenges When Using NH_3 as Fuel

Toxicity: NH_3 is toxic and poses safety risks during handling and transport.

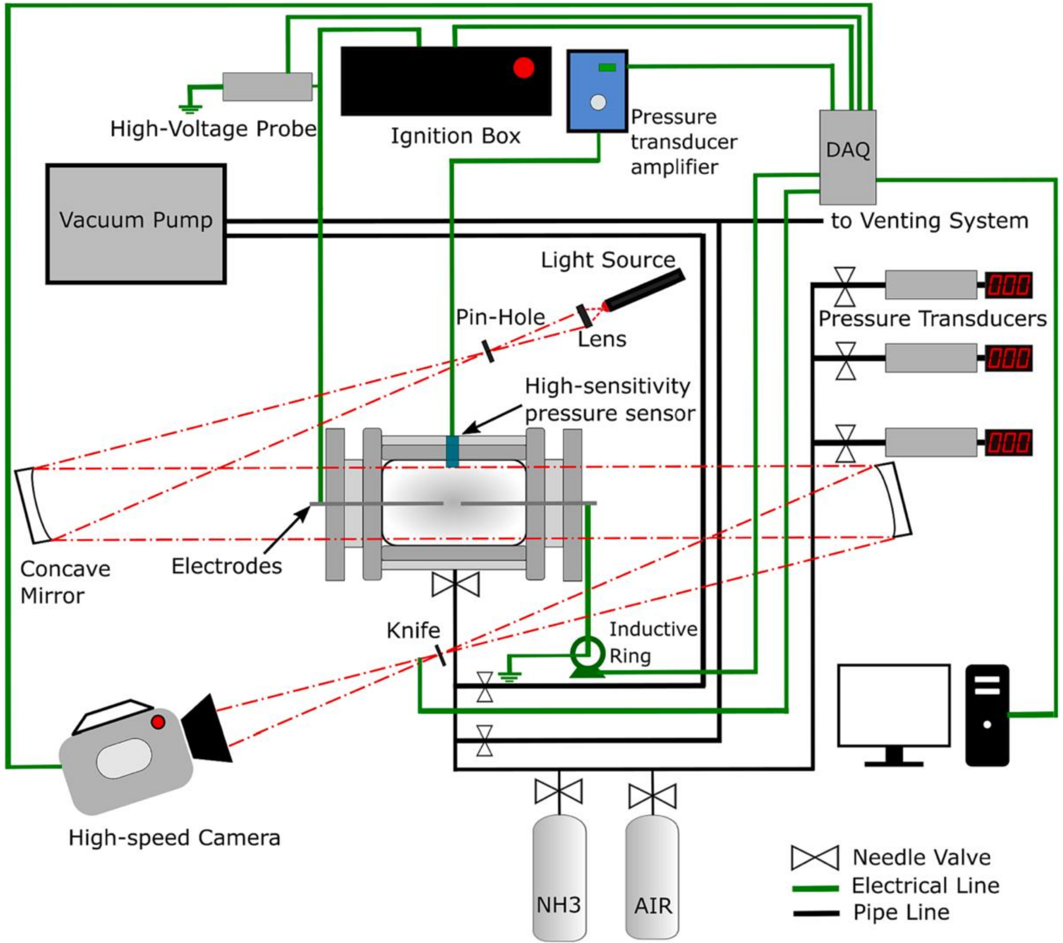
Combustion: NH_3 has limited flammability range, elevated ignition temperature, elevated heat of vaporization, lower laminar flame speed and lower energy output compared to traditional fuels.

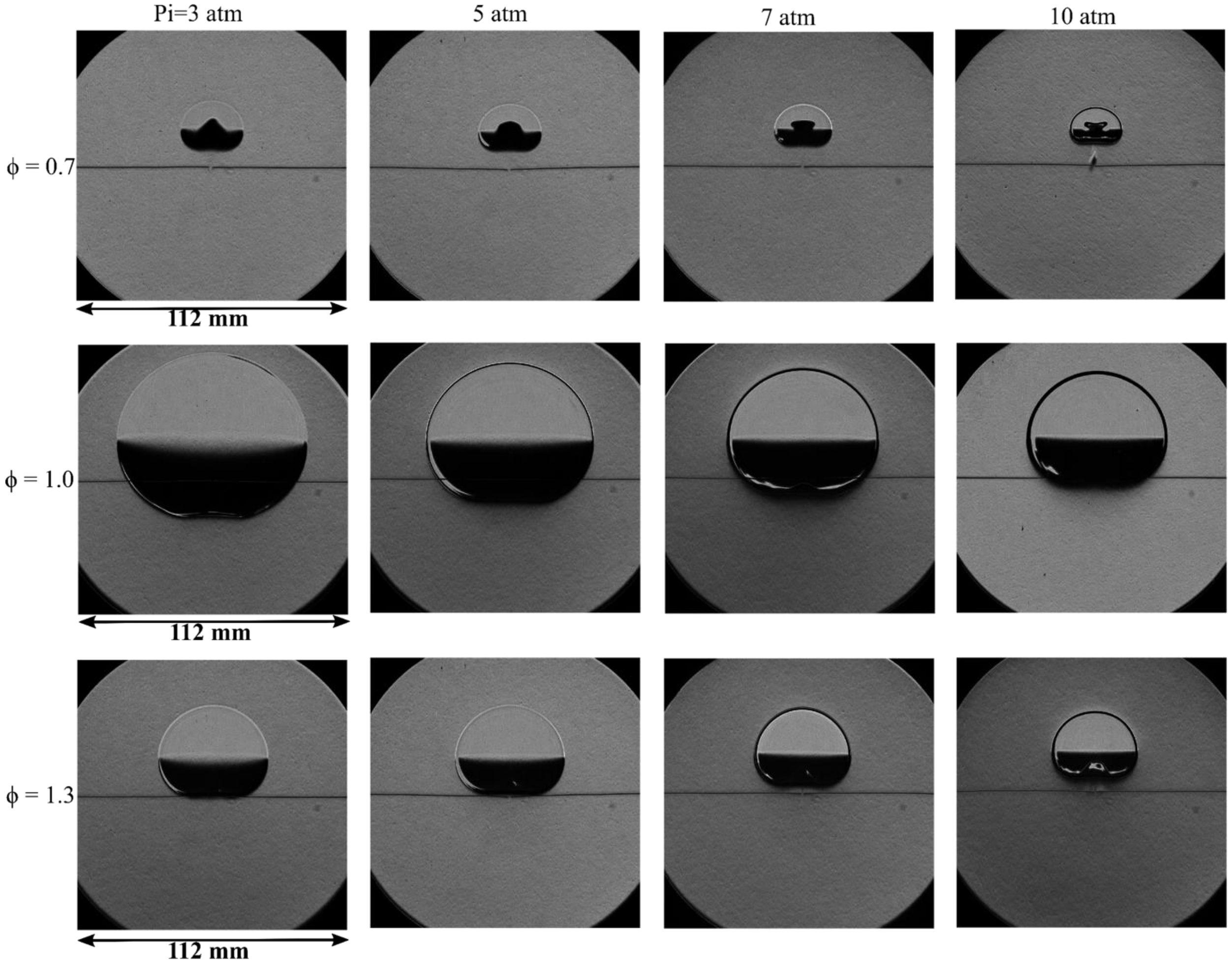
Emissions: NH_3 combustion produce nitrogen oxides (NO_x) and nitrous oxide (N_2O; high global warming potential), therefore requiring advanced emission control technologies. Currently, there are no binding regulations for NH_3 emissions if NH_3 is used as a fuel.

Atmospheric Pollution: NH_3 is a key precursor for the formation of atmospheric secondary inorganic particles, such as ammonium nitrate and sulfate. Limited information on the possible effect on the atmospheric concentration of gaseous NH_3 if NH_3 is used as a fuel.

Laminar Burning Velocity of NH_3/Air Mixtures at High Pressures

Currently, this is the only study that measured LBV of NH_3/air mixtures at 10 atm[1]

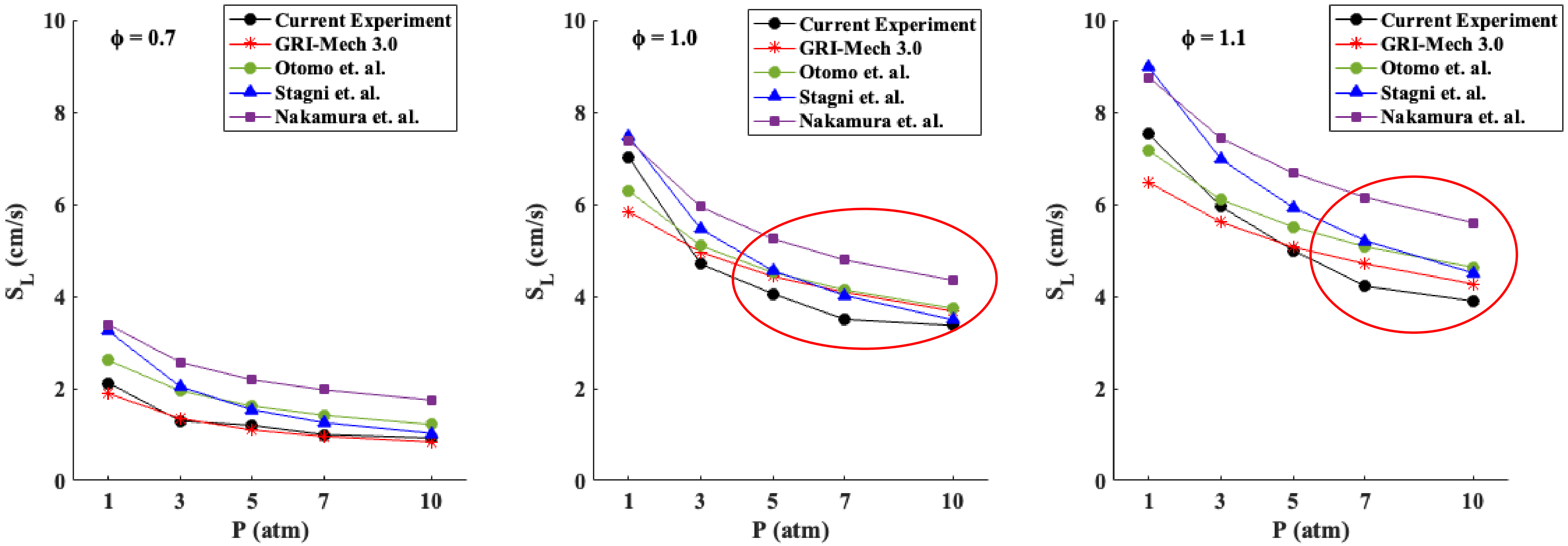




Schlieren images of NH_3/air flames at various initial pressures and stoichiometry 110 ms after ignition

[1] Alvarez, L. F., Shaffer, J., Dumitrescu, C. E., and Askari, O. Fuel 363, p. 130986, 2024.

Laminar Burning Velocity of NH_3/Air Mixtures at High Pressures

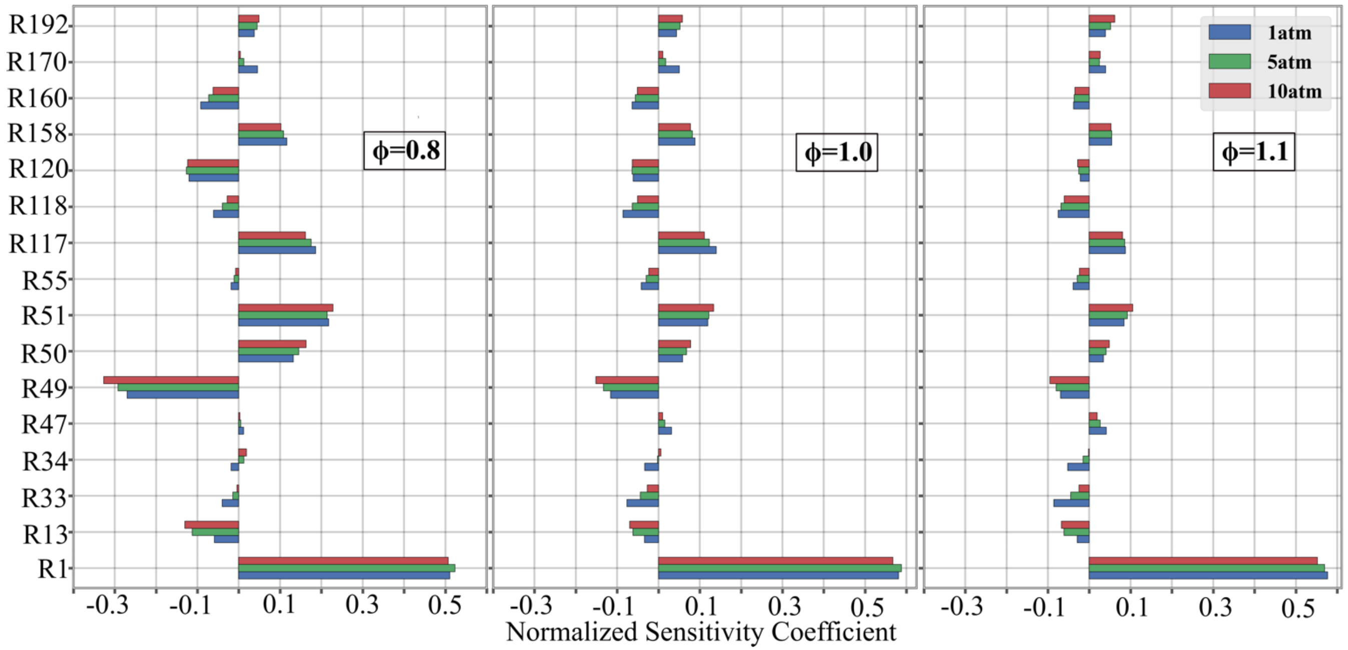


- LBV measurements were compared with existing detailed reaction mechanisms
- Numerical simulations for higher pressure suggested higher LBV values at equivalence ratio φ = 1.0 and φ = 1.1

Alvarez, L. F., Shaffer, J., Dumitrescu, C. E., and Askari, O.
Fuel 363, p. 130986, 2024.

Laminar Burning Velocity of NH_3/Air Mixtures at High Pressures

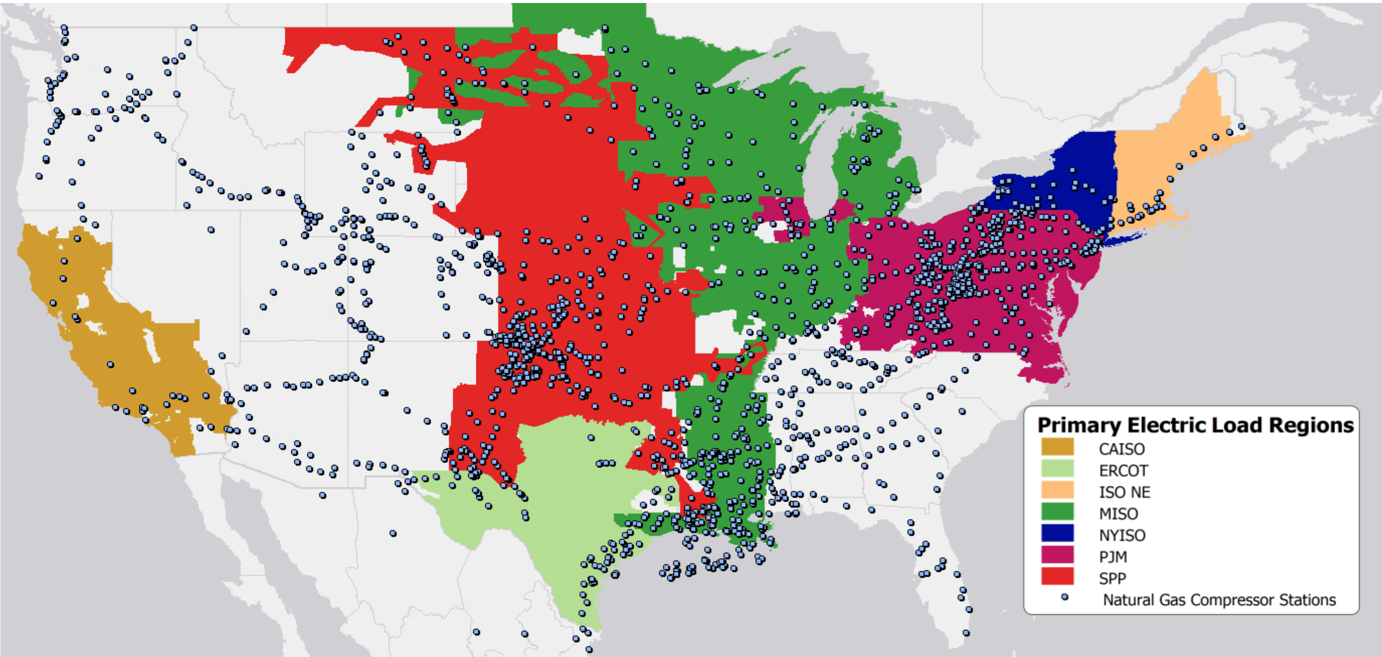
Number	Reactions
R1	$H + O_2 \Leftrightarrow O + OH$
R13	$H + O_2\ (+M) \Leftrightarrow HO_2\ (+M)$
R33	$H + NH_2 \Leftrightarrow H_2 + NH$
R34	$NH_2 + O \Leftrightarrow H + HNO$
R47	$N + NH_2 \Leftrightarrow 2H + N_2$
R49*	$NH_2 + NO \Leftrightarrow H_2O + N_2$
R50*	$NH_2 + NO \Leftrightarrow H_2O + N_2$
R51	$NH_2 + NO \Leftrightarrow NNH + OH$
R55	$H + NH \Leftrightarrow H_2 + N$
R117	$H + NO\ (+M) \Leftrightarrow HNO\ (+M)$
R118	$H + HNO \Leftrightarrow H_2 + NO$
R120	$HNO + OH \Leftrightarrow H_2O + NO$
R158	$N_2O\ (+M) \Leftrightarrow N_2 + O\ (+M)$
R160	$H + N_2O \Leftrightarrow N_2 + OH$
R170	$NH + NH_2 \Leftrightarrow H + N_2H_2$
R192	$N_2H_2 \Leftrightarrow H + NNH$



- Sensitivity analysis to understand the chemical reactions that impact the most the LBV of NH_3/air flames
- Competing reactions have a substantial impact on the oxidation pathway, with experimental conditions determining which reaction is dominant (i.e., which reaction promotes or inhibits the LBV)

Alvarez, L. F., Shaffer, J., Dumitrescu, C. E., and Askari, O.
Fuel 363, p. 130986, 2024.

NH_3 Can Replace Diesel or Natural Gas in Land-Based Off-Road IC Engine Applications



The majority of gas pipeline infrastructure in the U.S. will continue to rely on existing pipeline and compression capacity for the next several decades. Extra 8,000 MW needed if converted to electricity.[1]

Convert natural gas pipeline diesel-fired or natural gas-fired compression to ammonia-fired compression.

---

[1] ICF Resources, 2024, https://ingaa.org/wp-content/uploads/2024/01/Assessment-of-Electric-Drive-Compressor-Conversion1.pdf

NH_3 Use in Heavy-Duty CI Engines

Guidance on the safe design and operation of ammonia systems depends on jurisdiction

International design and maintenance rules and standards are needed.

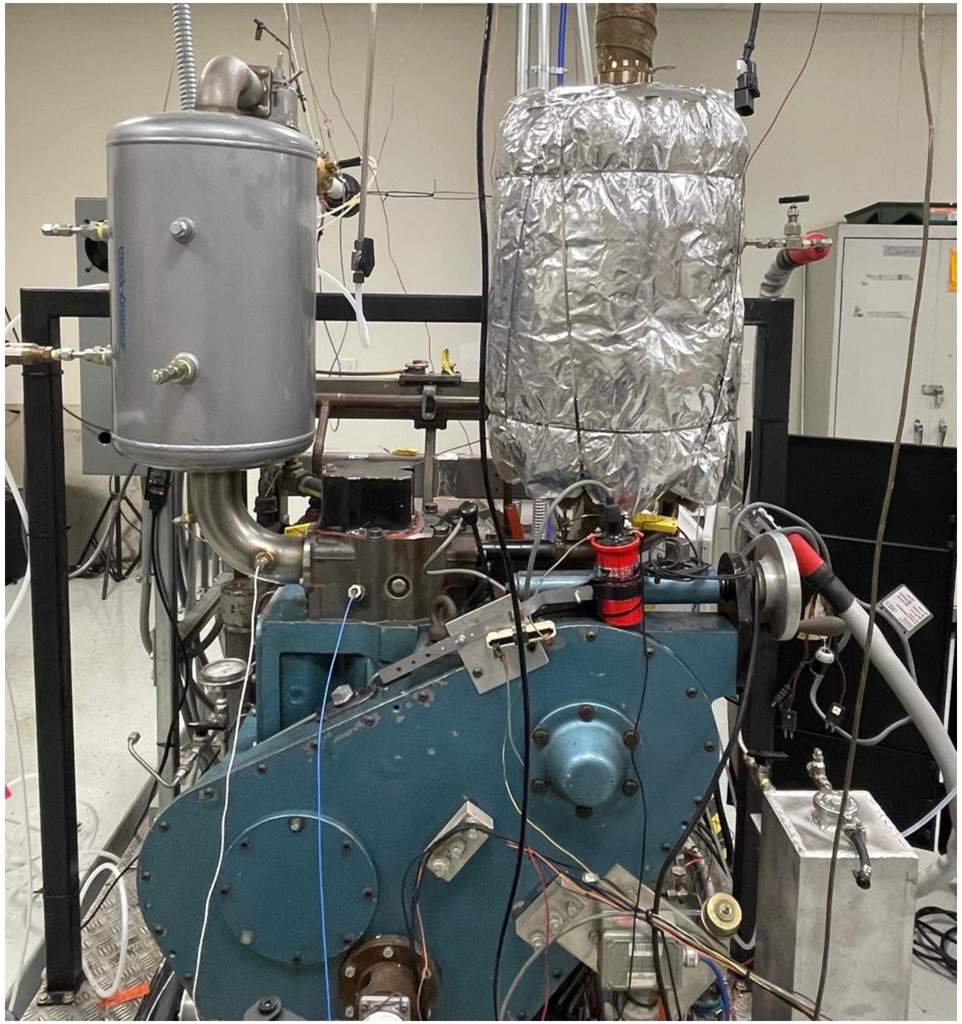
NH_3 dissolves in and/or react with engine oil.

How does it affect lubricant degradation? Are there potential health risks from exposure to contaminated oil during engine maintenance or when handling used oil?

High-temperature corrosion of engine components exposed to NH_3

Do we need to change seals, bearings, etc.?

NH_3 Use in Heavy-Duty CI Engine Converted to SI



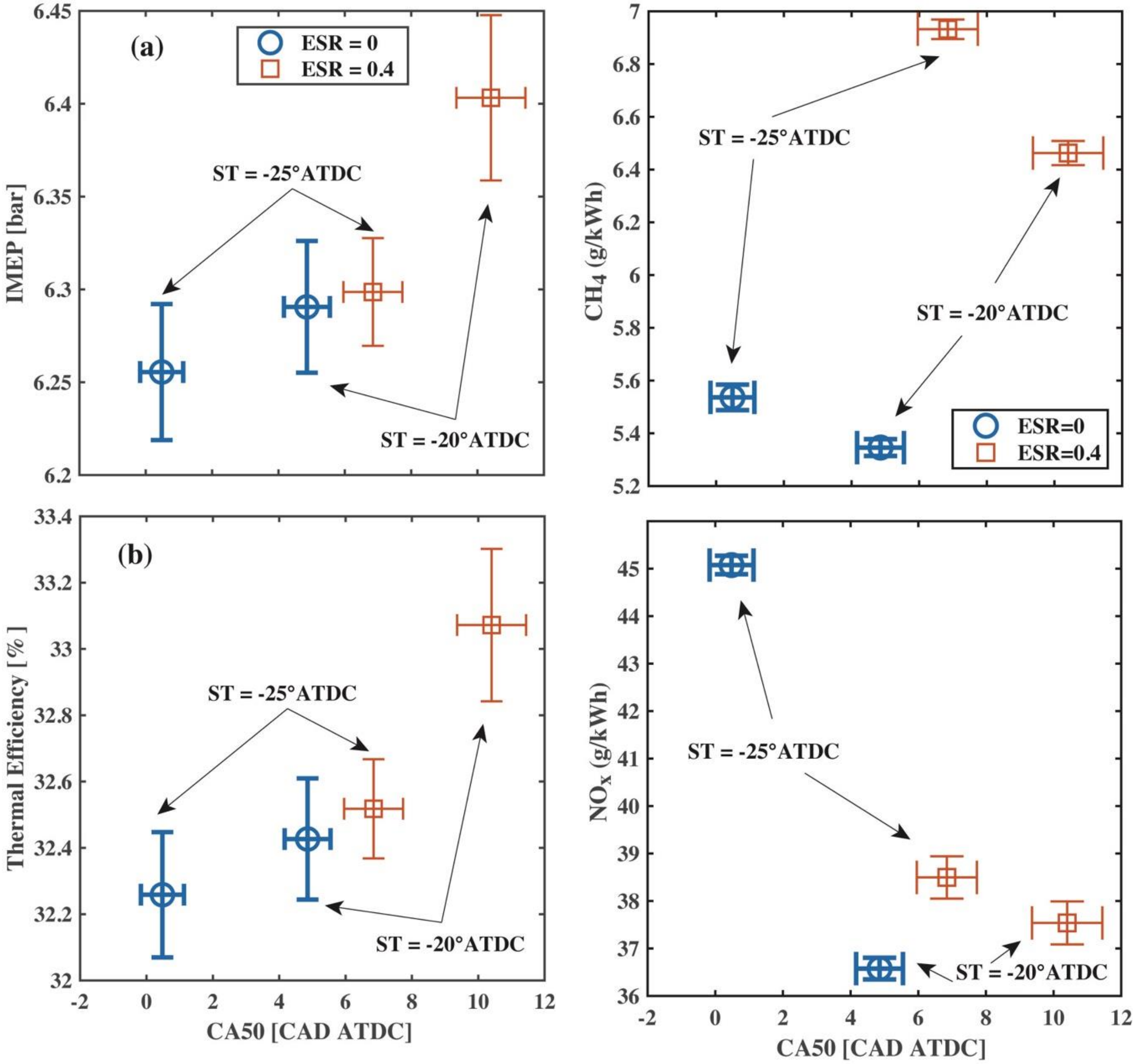
Displaced volume	1997 cc
Stroke	150 mm
Bore	130.2 mm
Connecting Rod	275 mm
Compression ratio	13.3:1
Number of Valves	2
Exhaust Valve Open	126 CAD ATDC
Exhaust Valve Close	10 CAD ATDC
Inlet Valve Open	12 CAD BTDC
Inlet Valve Close	140 CAD BTDC

Research on this engine platform is focused on **lean operation**

- Previous studies using NG as fuel serve as baseline
- Lower *dP/dt* means higher loads are possible

No optimization compared to previous studies except the addition of a better ignition system

Partially Replace Methane with NH_3



φ = 0.85, N = 900 RPM

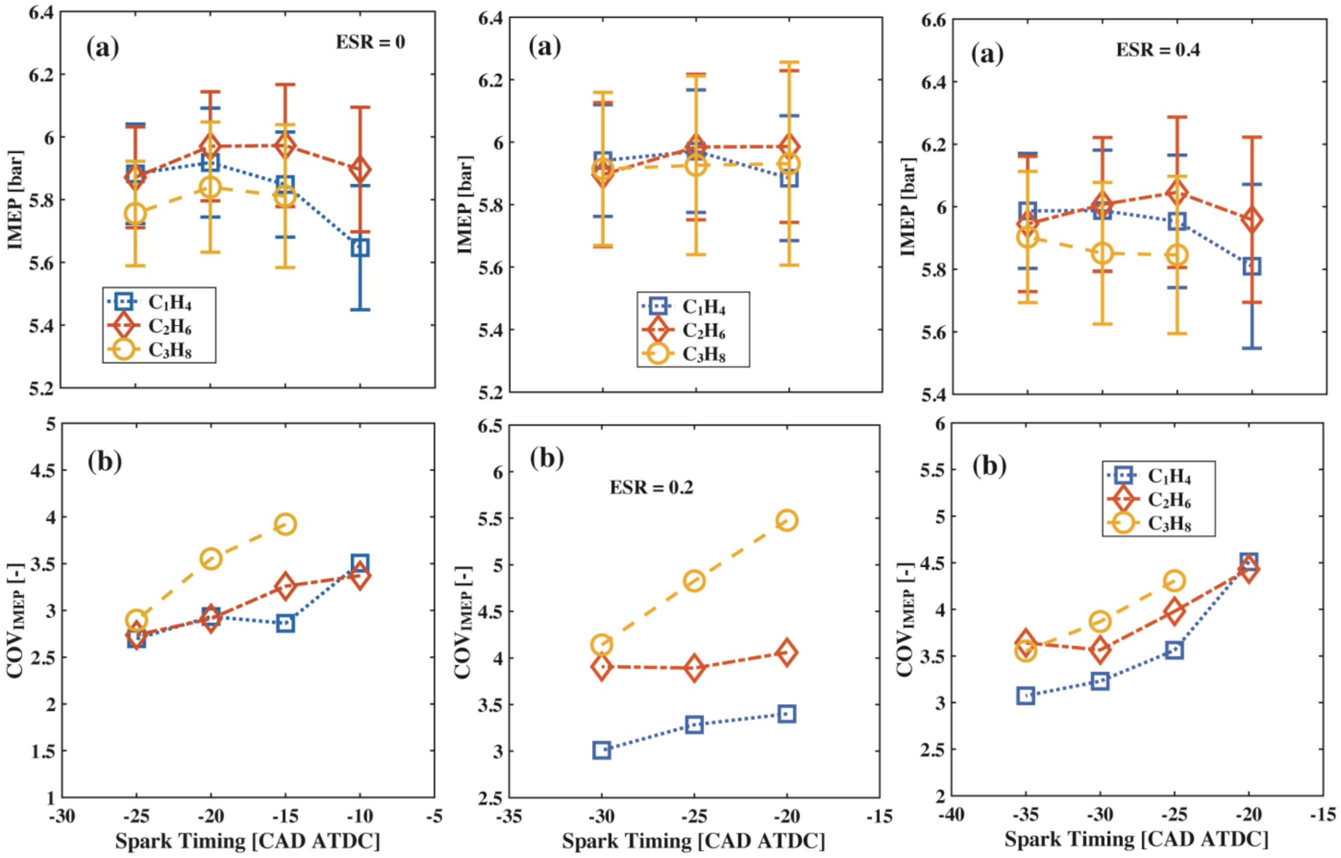
$$ESR = \frac{\dot{m}_{NH_3} LHV_{NH_3}}{\dot{m}_{CH_4} LHV_{CH_4} + \dot{m}_{NH_3} LHV_{NH_3}}$$

- Run the engine at the maximum possible ESR without any significant changes in engine control strategy other than just a spark timing adjustment
- Stable combustion
- No penalty in IMEP when NH_3 replaced CH_4
- $IMEP_{max}$ at same spark timing (ST) for both ESR cases (i.e., no need for changes in the engine control strategy).
- In-cylinder turbulence offset lower LBV of NH_3
- ESR = 0.4 had more optimum combustion phasing
- Similar NO_x emissions

WestVirginiaUniversity

Alvarez, L. F., and Dumitrescu, C. E.
SAE Technical Paper 2024-01-2371, 2024

Partially Replace Methane, Ethane, and Propane with NH_3



φ = 0.8, N = 1,000 RPM

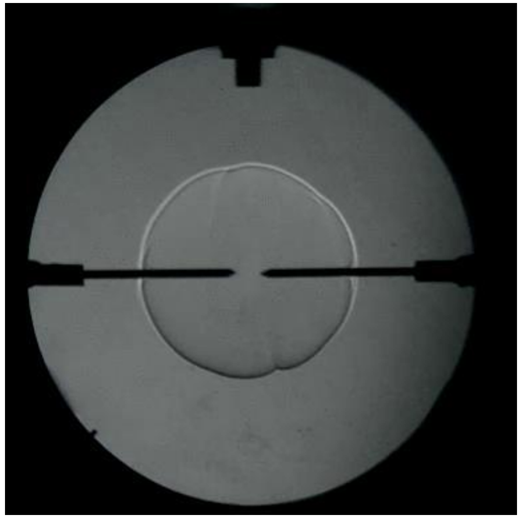
$$ESR = \frac{\dot{m}_{NH_3} LHV_{NH_3}}{\dot{m}_{C_xH_y} LHV_{C_xH_y} + \dot{m}_{NH_3} LHV_{NH_3}}$$

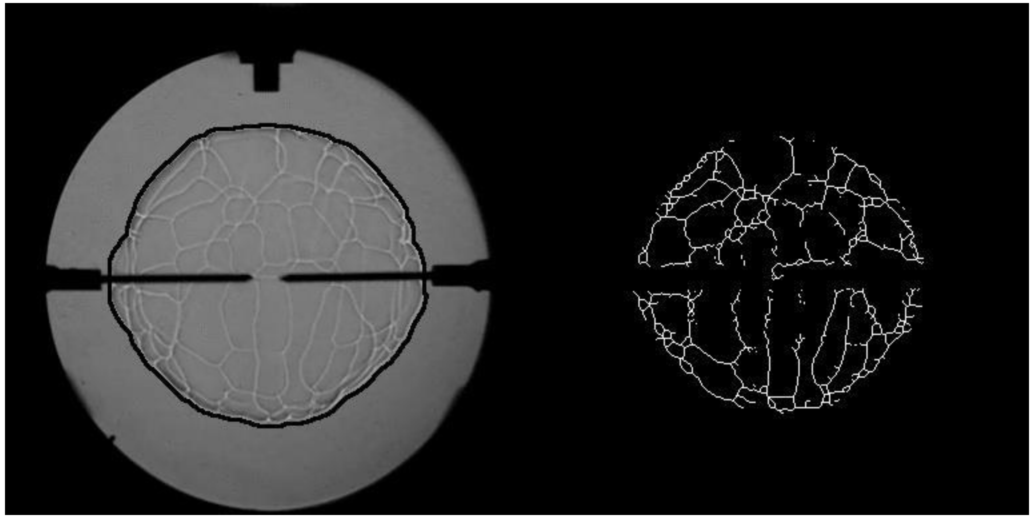
- Higher ESR increased COV$_{IMEP}$ but stable combustion
- No penalty in IMEP when NH_3 replaced NG components
- IMEP values were similar for different ST
- The increase in ESR lowered initial flame propagation rate but the combustion phasing was better
- The superposition of the IMEP error bars for all the three fuels at all the ESR conditions showed the engine capability to operate with a higher proportion of ethane or propane in the natural gas.

Alvarez, L. F., Askari, O., and Dumitrescu, C. E., Proc. ASME ICE2024,
Paper # ICEF2024-140567. San Antonio, TX, October 20-23, 2024.

NH_3/H_2 Blends – Effect of H_2 Concentration - CVCC

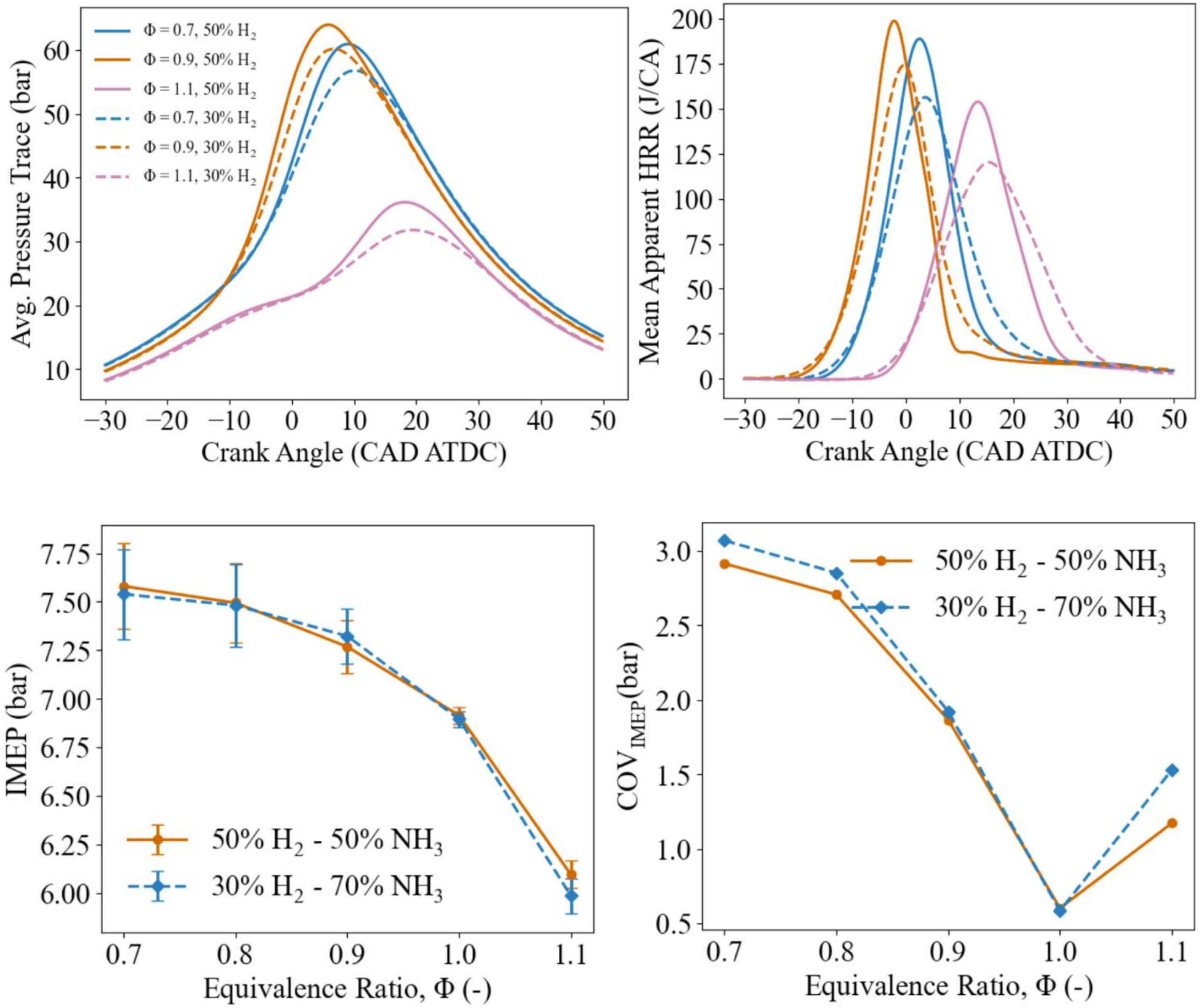
Wrinkled vs smooth spherical flames →





- Flame wrinkling can affect combustion, including the burning velocity, in turn affecting performance and emissions.
- Higher H_2 blend concentrations increase L_{crack}. The increase was faster and earlier (i.e., at smaller radii), which accelerated crack length growth.
- The maximum number of cracks become increasingly smaller at higher φ, even at higher blend fractions of H_2.
- The tendency of more instabilities at higher H_2 fractions and lower φ is consistent with how pure H_2-air spherical flames behave.

NH_3/H_2 Blends – Effect of Blend Concentration – SI IC Engine



- Higher H_2 percentage increased peak in-cylinder pressure and heat release in the SI engine.
- Peak in-cylinder pressures became higher as φ increased.
- Higher H_2 percentage reduced the burn duration (degrees of crank angle between 10% and 90% of cumulative heat release) due to the higher burning velocity of H_2 compared to NH_3.
- However, there was no indication that any of these metrics were due to increased flame wrinkling (which would have become apparent in COV_{IMEP} changes for different blend composition).

J.H. Mack, B. Nawaz, N. Nasim, S. Das, L. Alvarez, C. Dumitrescu,
Poster Session 2, THIESEL, September 12, 2024.

Research in Progress at West Virginia University

Successfully run 100% neat NH_3 without any engine optimization (look for published paper(s) soon)

IMEP for 100% neat NH_3 was comparable to NG operation as same conditions.

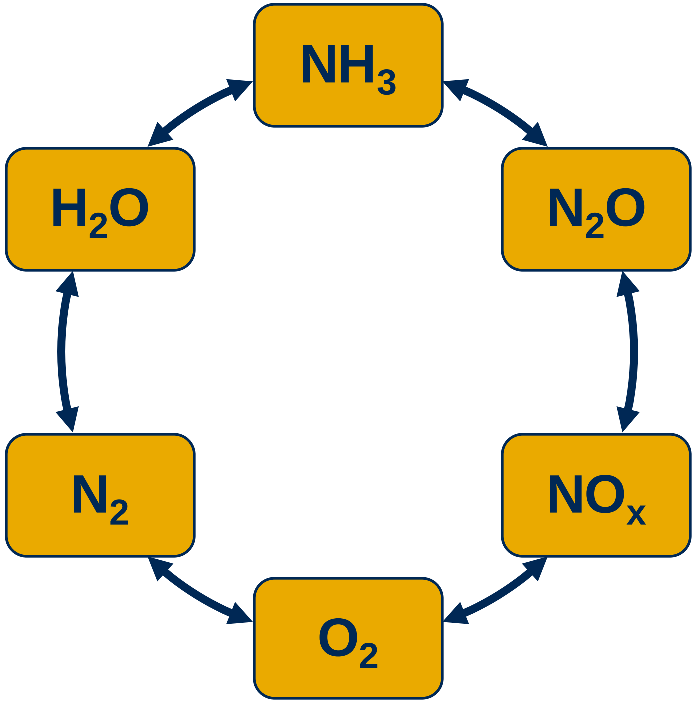
Highest IMEP was obtained at lean operation.

NH_3 is sticky and volatile. It is not easy to measure engine-out emissions and NH_3 leaks must be monitored.

NH_3 emissions in real exhaust gas can reach 1 vol% (10,000 ppm) or more.

Effect of equivalence ratio on NH_3, NO_x, and N_2O emissions is not straightforward (see next slide).

Aftertreatment Technologies for NH3 IC Engines[1]



$$4NH_3 + 3O_2 \rightarrow 2N_2 + 6H_2O$$

- Unique catalyst operating conditions present significant challenges to their direct application in NH_3 IC engines. Achieving efficient low-temperature conversion of N_2O (around 350°C) within the complex NO_x, N_2O, NH_3, O_2, and H_2O exhaust gas mixture is particularly demanding.
- Inhibitory effects of H_2O, O_2, and the optimal NH_3 feed add to emissions conversion complexity. Additionally, the high levels of H_2O vapor in NH_3-engine exhaust increase the hydrothermal aging of the catalyst, adversely impacting its long-term performance.
- NH_3 also oxidizes to N_2O and NO:

$$2NH_3 + 2O_2 \rightarrow N_2O + 3H_2O$$
$$4NH_3 + 5O_2 \rightarrow 4NO + 6H_2O$$

- Noble metals aggravate N_2O emissions.

1Cano-Blanco DC., Elsener M., D'Alessandri J., Peitz D., Ferri D., Kröcher O., The Journal of Ammonia Energy 02 (2024) 064–072

West Virginia
Higher Education
Policy Commission

Chemical
Alliance
ZONE
West Virginia

UMASS
LOWELL

WestVirginiaUniversity.

AVN

WEST VIRGINIA STATE
UNIVERSITY
1891

WestVirginiaUniversity.
COLLEGE OF BUSINESS AND ECONOMICS
Bureau of Business and Economic Research

CONCORD U

Thank you!

Questions?