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Advancing Cleaner Aviation Fuels: NH_3-SAF intermediate mixtures

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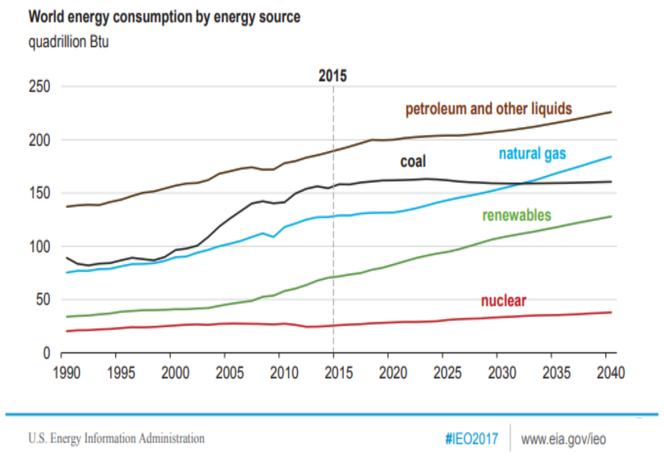
ENERGY TRANSITION SCENARIO



Energy consumption is going to increase for all traditional fuels other than coal

Problem statements

- The exhaustion of traditional fossil fuels → **Break the dependence on them**
- Associated GHG emission → **Go towards a decarbonization of energy**
- Emission of hazardous and unpleasant air pollutants (soot, NO_x, SO_2…) → **Optimize a process while meeting with the pollutant emission standards**

LOW-CARBON AVIATION CHALLENGE

Ammonia

Ammonia is a carbon-free fuel but presents combustion challenges

Sustainable Aviation Fuels (SAFs)

SAFs are essential but their combustion chemistry is not fully understood

NH_3/SAF blends could combine the advantages of both fuels

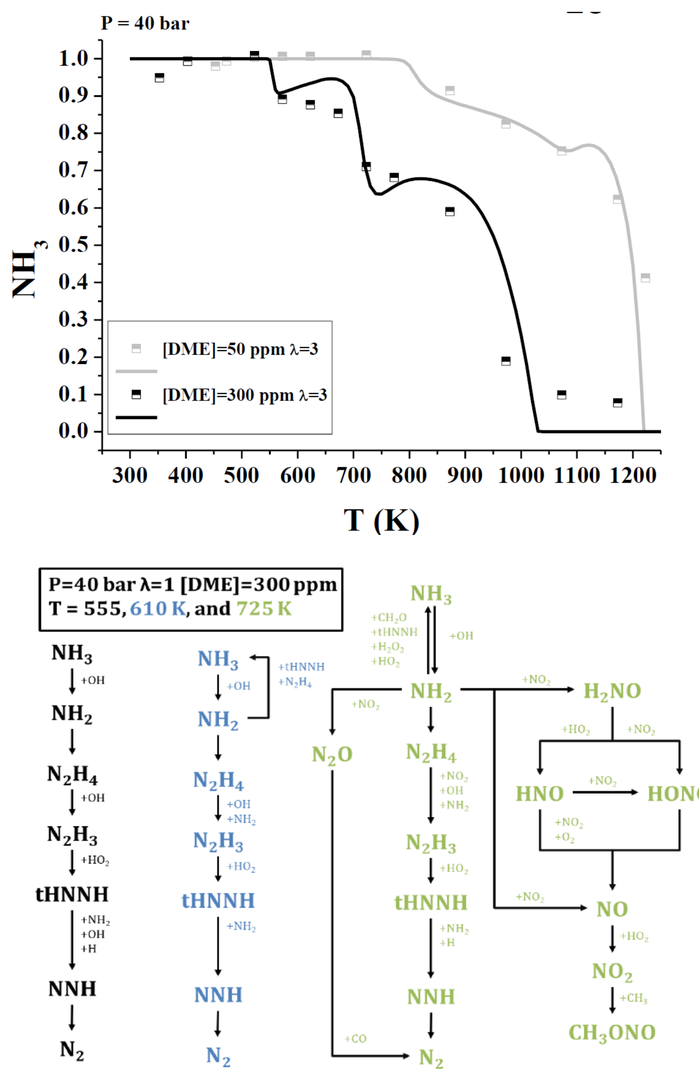
"DUAL FUEL APPROACH"

✓ Mixing ammonia with other fuels can enhance NH_3 combustion properties

✓ N_2O is the main nitrogen oxide generated when ammonia is burned in the presence of carbon containing fuels and/or at high pressures

PREVIOUS WORKS

e.g. High-pressure conversion of ammonia additivated with dimethyl ether in a flow reactor
[*García-Ruiz et al. Combust. Flame 2025*]



GENERAL PURPOUSE

To investigate the conversion of ammonia mixtures with key intermediate compounds generated during the combustion of Sustainable Aviation Fuels (i.e. acetaldehyde, acetone, and acetic acid) under high-pressure conditions

Specific Objectives

✓ **Investigate** the high-pressure conversion of NH_3/acetone, NH_3/acetaldehyde, and NH_3/acetic acid mixtures

✓ **Assess** the effects of operating conditions (temperature, pressure, and oxygen stoichiometry) on fuel conversion and pollutants formation

✓ **Develop and validate** a detailed kinetic reaction mechanism based on experimental data

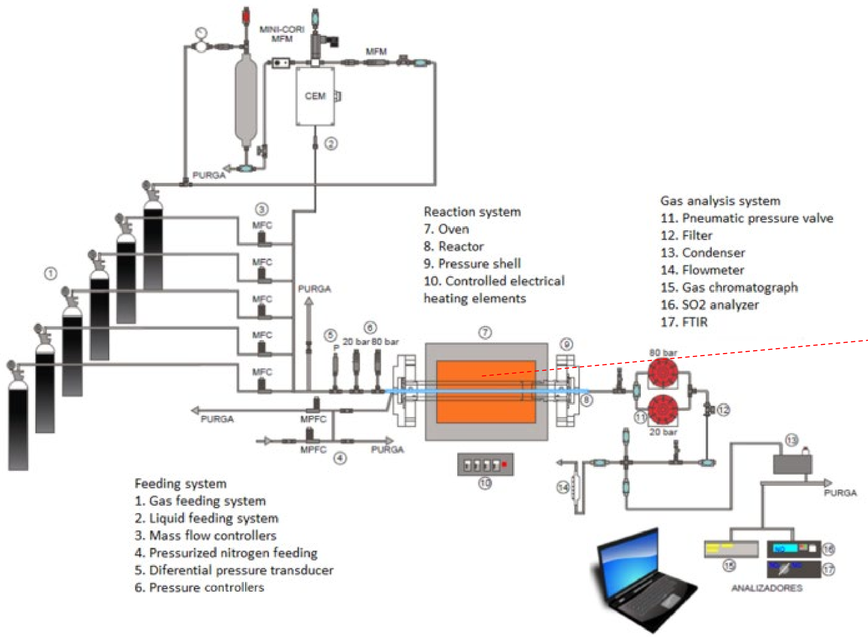
The conversion of SAFs, whether in oxidation or pyrolysis, generates a variety of intermediate species depending on the fuel's chemical composition and operating conditions (temperature, pressure, stoichiometry, etc.) [*Gong et al. J. Energy Inst. 2021*]

Key Intermediates from SAFs like terpenes include oxygenated compounds such as **aldehydes, ketones and carboxylic acids** [*Dbouk et al. Fuel 2024*]

METHODOLOGY

Experimental: Laboratory scale flow reactor experiments
Simulation: Run in Chemkin-Pro

EXPERIMENTAL: High pressure set-up



Quartz tubular Flow reactor
Reaction zone:
45 mm inside –
900 mm in length
Temperatures up to 1200 K
Pressures up to 50 bar

COMPUTATIONAL MODELING

Calculations - Software Chemkin-Pro
[*CHEMKIN-PRO 15131. Reaction Design, 2013*]

Reaction Mechanism

Elemental reactions and their rate parameters:

$$k_{fi} = A_i T^{\beta_i} \exp\left(\frac{-E_i}{RT}\right)$$

Thermodinamic data base

Plug-flow reactor code

Source of Inlet1 → C1_PFR → C1_Product

Process conditions
Temperature
Pressure
Residence time
Reactant concentrations

Output Results

-Product concentrations

- Sensitivity analysis

- Reaction rate analysis

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