ALFA

Ammonia as a Liquid for the Future of Aviation

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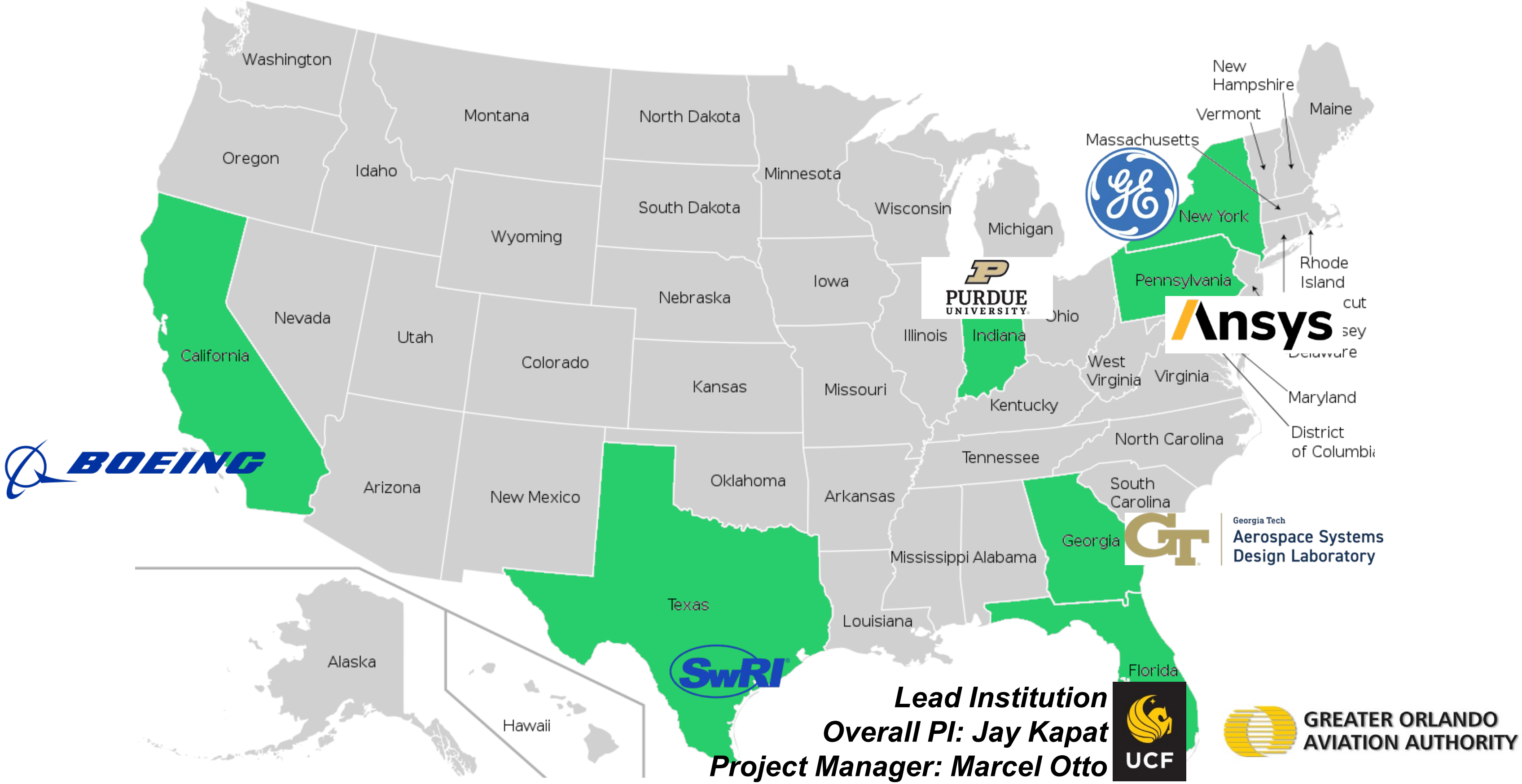
Funded Through NASA ARMD *University Leadership Initiative*
Under Strategic Thrust – Zero Emission Aviation

November 16, 2022

The Team



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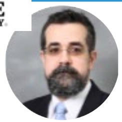
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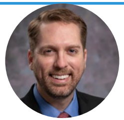

Tim Allison

+ Non-Advocate Peer Review Board

Background & Rationale
Why this approach?

Why Ammonia for Decarbonization of Aviation?

- When NASA asked for proposals under the thrust area “Zero Emission Aviation”

- We asked ourselves what is meant by “Zero Emission Aviation”.

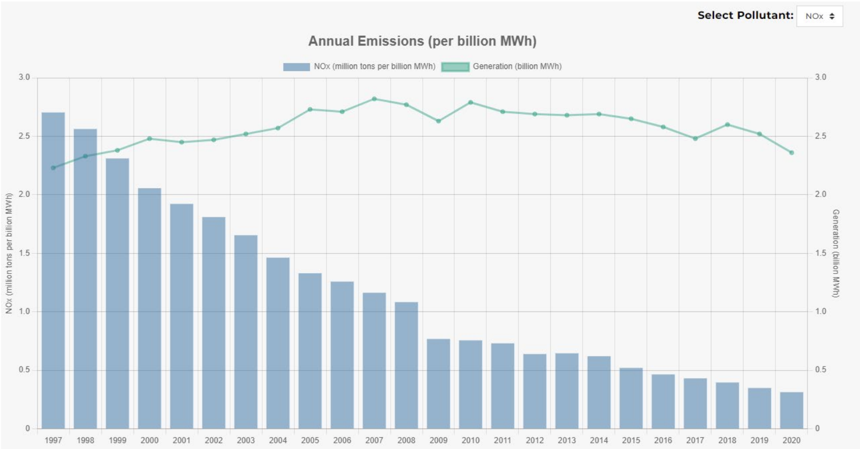
- Should we aim for:
    - Zero carbon aviation ?
    - “Net-zero” aviation ?
    - Zero emission of all kinds ?

CO_2 (g/s), cruise	~1800
NOx (ppm)	~200
H_2O (g/s), cruise	~750
NVPM[1] ($\mu g/m^3$)	475

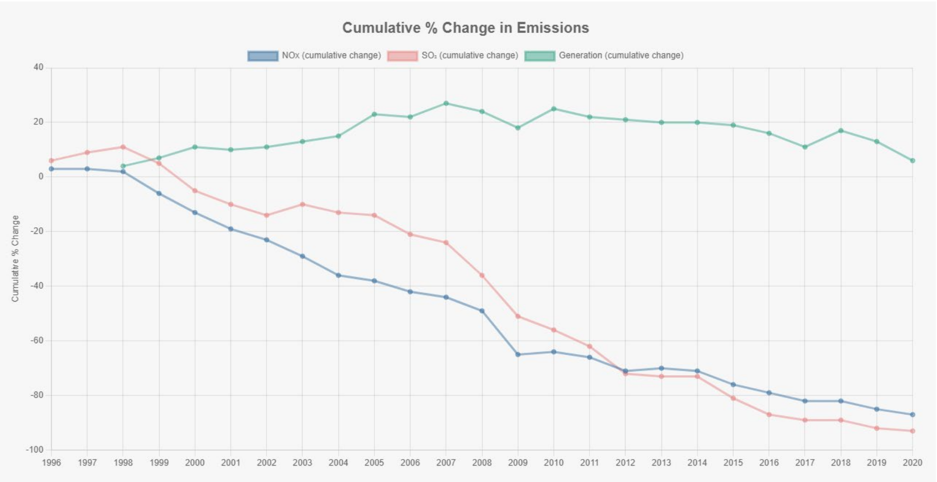
- We approached the project with the objective of eliminating, or at least minimizing, emission of ***all kinds*** in the ***engine exhaust***:
    - CO_2
    - NOx (Note: 100-year GWP for N_2O = 265; significant ODP)
    - H_2O (contributes to contrails that cause radiative forcing)
    - NVPM (leads to higher contrail formation)

NOx minimization - Let us learn from Power Generation

"Power Generation NOx Tracker" https://www.cecs.ucf.edu/nox/ Supported by Mitsubishi Power



University of Central Florida engineers—who specialize in power generation—collected the data from an Environmental Protection Agency database to create the tracker and website. The chart shows the annual amount of NOx emission per MWh. A continuous downward trend can be observed over the past few decades.



$$2NO + 2NH_3 + \frac{1}{2}O_2 \xrightarrow{catalyst} 2N_2 + 3H_2O$$

$$2NO_2 + 4NH_3 + O_2 \xrightarrow{catalyst} 3N_2 + 6H_2O$$

- Too much ammonia injection can lead to ammonia emission, referred to as "ammonia slip"

Competing Technologies

Safety?
Water in Production?

Adapted from: McKinsey, 2020, "Clean Skies for Tomorrow: Sustainable Aviation Fuels as a Pathway to Net-Zero Aviation," World Economic Forum, www3.weforum.org/docs/WEF_Clean_Skies_Tomorrow_SAF_Analytics_2020.pdf

Kerosene Baseline	Battery-electric	H2 fuel cell only	H2 turbine	SAF	NH3
Climate Impact (integrated)	100% reduction	75-90% reduction	50-75% reduction	30-60% reduction	50-99% reduction
NO_x only	0	0	Potential increase	Same	Almost 0
Aircraft Design	Battery density limits range to 500-1000km	Feasible only for commuter to short-range segments	Feasible for all segments except for flights>10,000 km	Only minor changes	Feasible for all segments except >5000 miles
Aircraft Operations	Same or shorter turnaround time, weight remains constant throughout a flight negatively impacting range	1-2x longer refueling times for up to short range, special safety standard	2-3x longer refueling times for medium to long-range; special safety standard	Same turnaround times	Same or marginally longer turnaround times
Airport Infrastructure	Fast-charging or battery exchange systems required	LH_2 distribution and storage with cryocooling are required		Existing infrastructure can be used	Needs NH_3 distribution and storage, no cryocooling
Global Supply Chain Concerns	Minimal – used in other applications	Supply interruption in Global Aviation		Quality uniformity and scaling, competing land use	Moderate – existing infrastructure (e.g., fertilizer)
Water in Exhaust	0	Yes		Yes	Minimized

GREATER ORLANDO AVIATION AUTHORITY

Ammonia is more than an Energy Carrier!

	Jet A	SAF
CO_2 (g/s), cruise	~1800	~1800
NOx (ppm)	~200	~200
NH_3 (ppm)	0	0
H_2O (g/s), cruise	~750	~750
NVPM[1] ($\mu g/m^3$)	475	>475

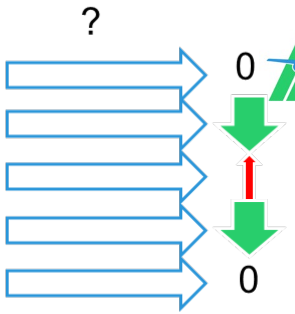


Table 2. Flame Characteristics of H_2 and NH_3

Fuel	H2	NH3
Max Lam Flame Speed (cm/s)	291	7
Adiabatic Flame Temp (K)	2400	2075
Flammability Range	0.1–7.1	0.6–1.4
Critical Temp (K), Pressure (MPa)	33, 13	405, 11.3
Triple Pt. Temp (K), Pressure (MPa)	14, 0.07	195, 0.006

Table 3. Comparison of Ammonia with Kerosene, Hydrogen and Methanol[12]

Properties	Unit	Kerosene	Hydrogen		Methanol	Ammonia
Stored as Temperature Pressure	- °C MPa	Liquid Ambient	Gas Ambient 69	Liquid - 252.9 Ambient	Liquid Ambient	Liquid -33 (or 25) 0.1 (or 0.99)
Density	kg/m^3	840	39	70.8	792	600
Explosive limit	%vol	0.7 to 5	4 to 75	4 to 75	6.7 to 36	15 to 28
LHV	MJ/kg MJ/L	43 35	120 4.5	120 8.49	20.1 15.8	18.6 12.7
H2 content	wt% $kg\text{-}H_2/m^3$	N/A N/A	100 42.2	100 70.8	12.5 99	17.8 121
Hydrogen release	-	N/A	Pressure release	Evapora-tion	Catalytic decomp @ Temp > 200 °C	> 300 °C
Energy to extract H_2 (g)	$kJ/mol\text{-}H_2$	N/A	-	0.907	16.3	30.6

Tech Challenges and Progress Monitors

Ammonia as a Liquid for the Future of Aviation

Tech Challenge I: Minimization of all Emissions

Challenge Definition: ***To Minimize*** NOx, NH3, and H2O concentration in the engine exhaust under cruise conditions.

The proposed innovation further eliminates emissions of carbon dioxide (CO2) and non-volatile particulate matter (NVPM), which are not tracked anymore. However, ammonia is now introduced and hence its emission is to be monitored and minimized.

Duration: Y1/Q1 to Y5/Q3

Progress Indicators:

(1) Concentration of NOx in the engine exhaust under cruise conditions, measured in ppm or parts per million - ***Success criterion***: 5ppm or less, at the end of the project

(2) Concentration of NH3 in the engine exhaust under cruise conditions, measured in ppm or parts per million - ***Success criterion***: 20ppm or less, at the end of the project

(3) Flow rate of H2O in the engine exhaust under cruise conditions, that is responsible for contrail formation, measured in g/s - ***Success criterion***: 500 g/s or less, at the end of the project

Tech Challenge II: Integration of new Components into Engine and Airframe

Challenge Definition: ***To Minimize*** adverse impact on engine/airplane operation when new components are integrated into the engine and airframe.

Progress Indicators: (1) Total payload decrease, (2) Realized Low Heating Value, (3) Start-up Time.

Tech Challenge III: Minimization of Aircraft and Infrastructure Upgrade and Operational Cost

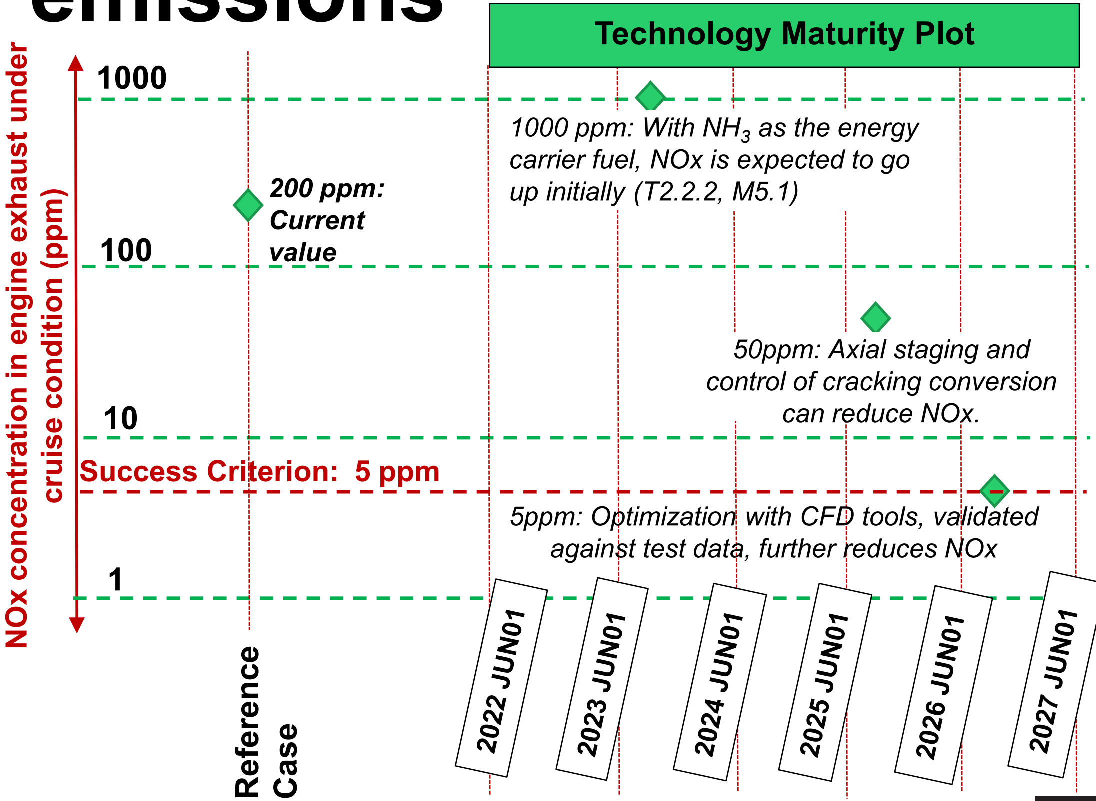
Challenge Definition: ***To Minimize*** the cost of upgrade and operation when new technologies are introduced to airports and airplanes.

Progress Indicators: (1) Total fuel cost compared to reference, (2) Airframe cost increase compared to reference, (3) Gate cost increase compared to reference, (4) Dollar per passenger mile increase compared to reference

TECH Challenge I: Minimization of all emissions

- *Progress Indicator*:
  - NOx concentration in engine exhaust under cruise condition

- Action Plan
  - Control with Axial staging and Mixture composition to reduce NOx under test conditions (T2.2.1, M10.1)
  - CFD code, validated against test data, shows lower NOx emission (T2.2.3, T2.2.4, M13.1)
  - Optimization of SCR, Selective Catalytic Reduction, to minimize both NOx and NH3 (T2.3.1, M16.1)
  - CFD optimization under cruise/engine conditions (T2.2.3, M17.1)



Progress Indicators Summary

- Three Tech Challenges
  - 3, 3, & 4 Progress Indicators each
- Continuously tracked throughout project
- Covering technical and economical aspects
- Task Deliveries feed directly into Performance Indicators and Tech Challenges

Selected Project Details

ALFA

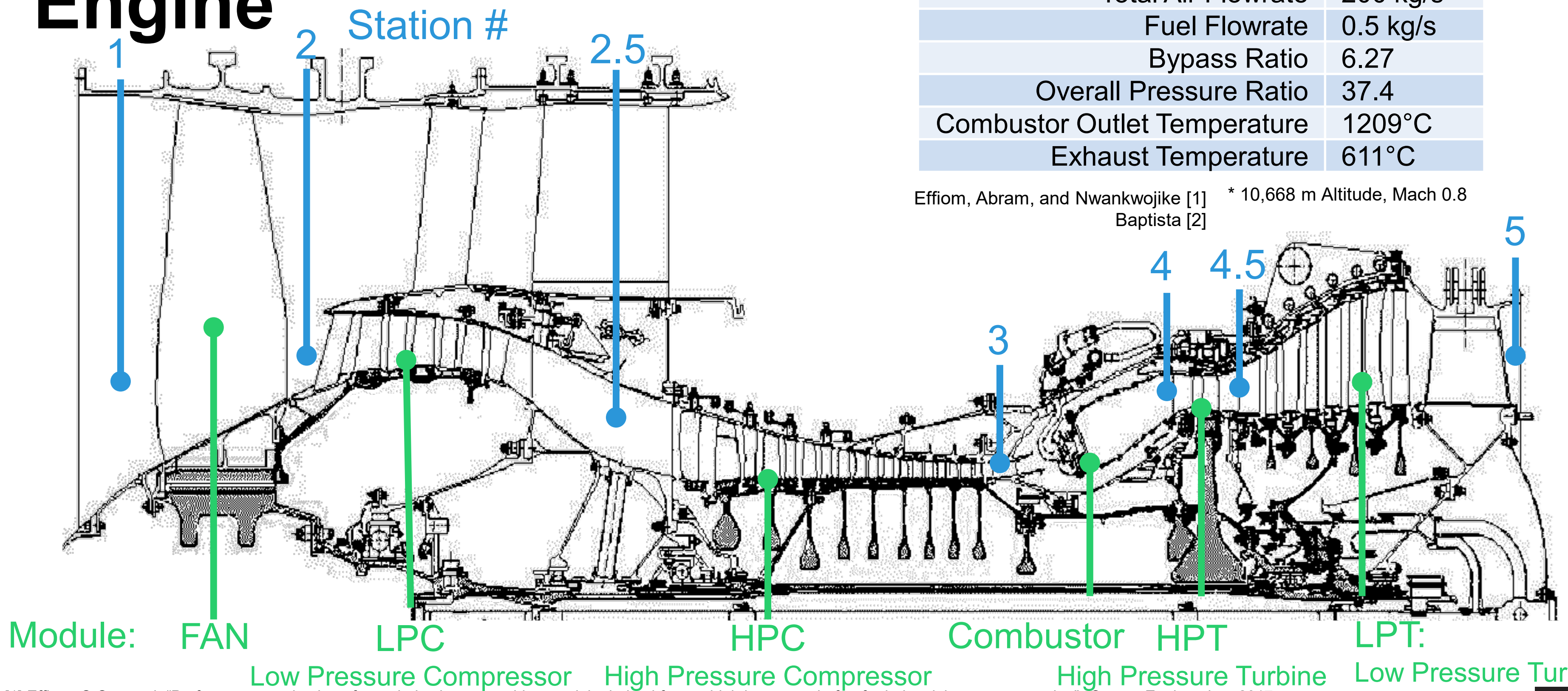
Ammonia as a Liquid for the Future of Aviation

Today's Narrow Body Jet Engine

Cruise Conditions*	Value
Engine Inlet Temperature	-54°C
Total Air Flowrate	200 kg/s
Fuel Flowrate	0.5 kg/s
Bypass Ratio	6.27
Overall Pressure Ratio	37.4
Combustor Outlet Temperature	1209°C
Exhaust Temperature	611°C

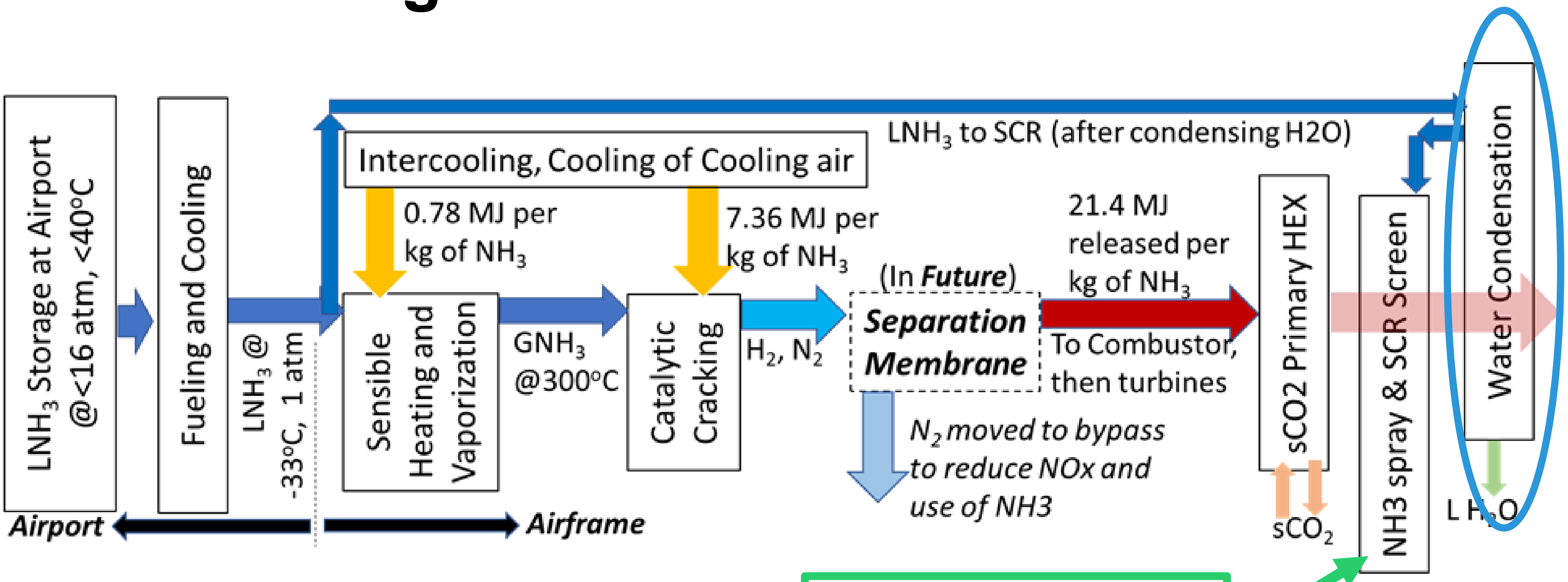
Effiom, Abram, and Nwankwojike [1]
Baptista [2]

* 10,668 m Altitude, Mach 0.8



[1] Effiom, S.O., et. al, "Performance evaluation of aeroderivative gas turbine models derived from a high bypass turbofan for industrial power generation", Cogent Engineering, 2017.
[2] Baptista, F.M.C., "A 0-d off-design performance prediction model of the CFM56-5B turbofan engine", Universidade de Lisboa, Portugal, 2017.

Multiple Purpose of Ammonia – Energy Carrier, Thermal management & NOx/H2O Control



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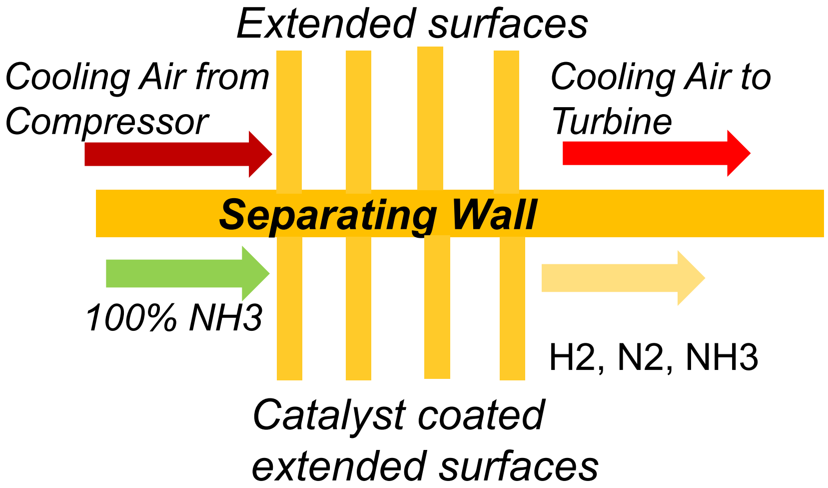
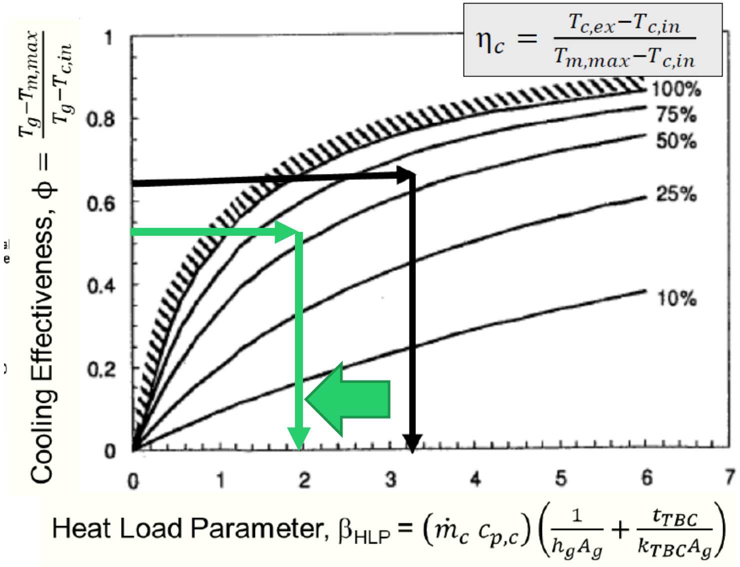
Cracking and Thermal Management

- Cracking is an endothermic process
- The heat needed for cracking can be used to cool the turbine cooling air
- Both processes (catalysis and heat transfer) are surface area dependent





- Extended surfaces on either side will be optimized through various means that have been applied by the group in the past, and can be fabricated through additive manufacturing
- This will lead to lower cooling air needs, giving better SFC

Three Avenues for Improved Performance

Compressor Intercooling

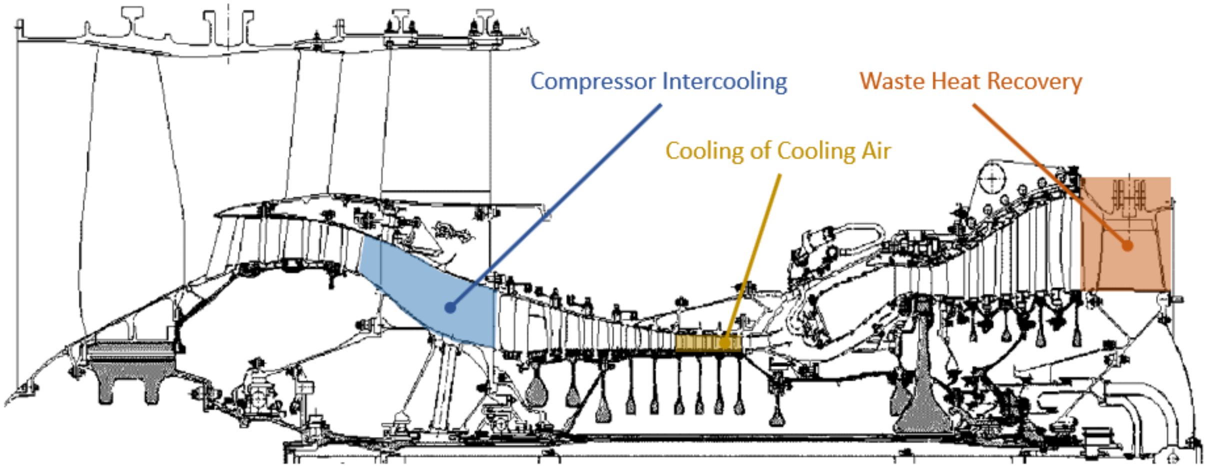
- NH3
- $Work = \int_{V_1}^{V_2} PdV$
  - $P \propto T \rightarrow Work \propto T$
  - Less Temperature → Less Work

Cooling of Cooling Air

- NH3
- $\Delta H_{air} + \Delta H_{NH_3} = 0$
  - $\Delta H_{fg,NH_3} \approx 1370 \frac{kJ}{kg}$
  - High cooling potential of NH3

Waste Heat Recovery

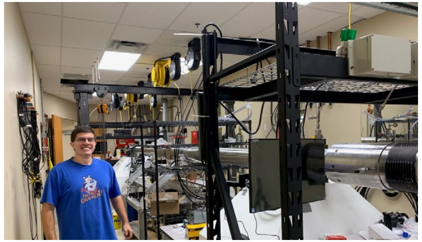
- sCO2
- $\eta_{ideal} = 1 - \frac{T_{Cold}}{T_{Hot}} \approx 55\%$
  - Potential for significant power extraction from exhaust heat

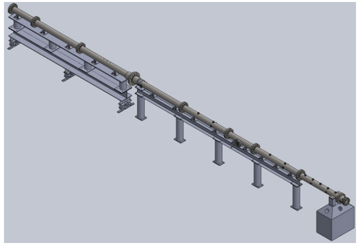


http://www.aircraftmonitor.com/

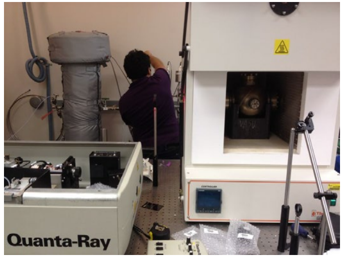
UCF's Experimental Facility for Probing NH_3/H_2 Kinetics

2 Shock Tubes – realistic GT conditions with H2/NH3 permits





Flame Speed Measurements



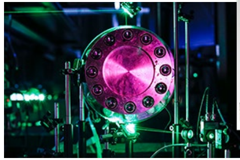
Capabilities

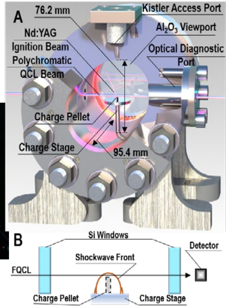
- High-Pressure Combustion up to 1000 bar and autoignition and emission species Measurements.
- Toxic impurities NOx, SOx, H_2S, and syngas
- Hydrogen or ammonia combustion with impurities
- Synthetic and biofuels
- Lasers for studying NOx formation routes
- High-Temperature Thermomechanical Response and Surface Chemistry of Novel Materials
- High -Pressure and -Temperature Molecular Spectroscopy Data for the Development of State-of-the-Art Non-Intrusive Optical Diagnostics

Planned Experiments

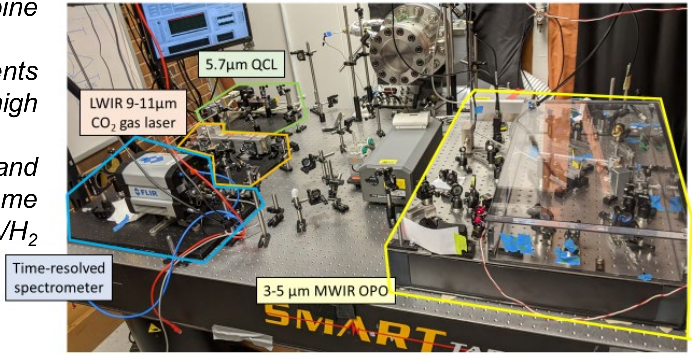
- *Autoignition delay and species time history measurements of NH_3/ H_2 mixtures at aviation turbine relevant conditions.*
- *Flame speed experiments with NH_3/H_2 mixtures at high pressures.*
- *Well stirred reactor and counterflow flame experiments for NH_3/H_2 mixtures.*

Laser and Optical Diagnostics

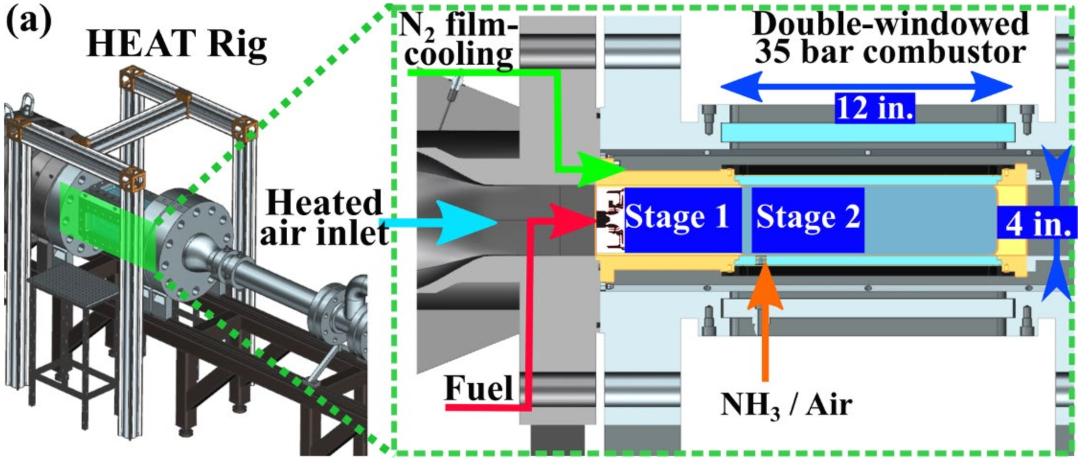


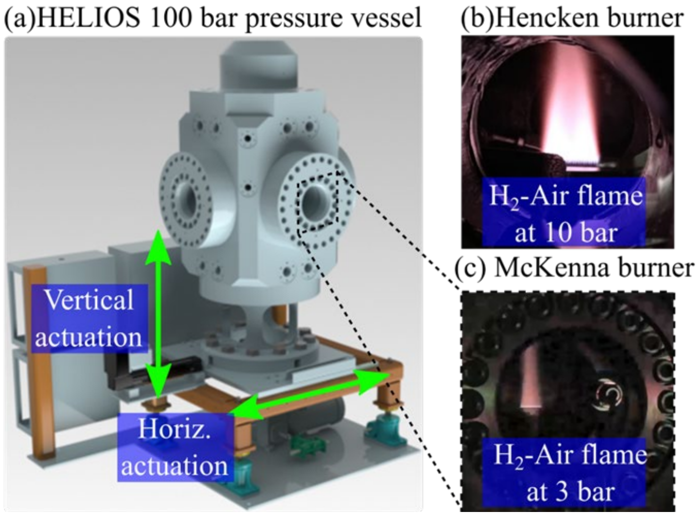


UCF Shock Tube Laser Diagnostics



Purdue – Experimental Validation under Engine Representative Conditions

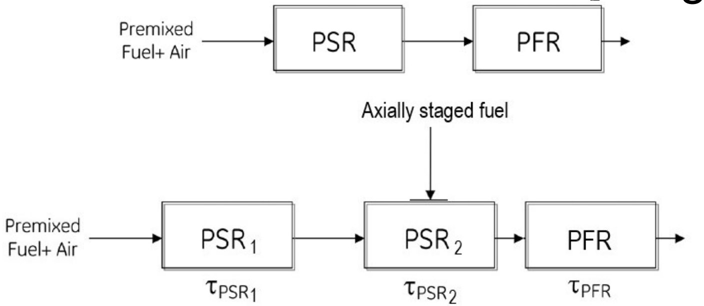




GE – Reactor Network Modeling and CFD Analysis for Emission Control

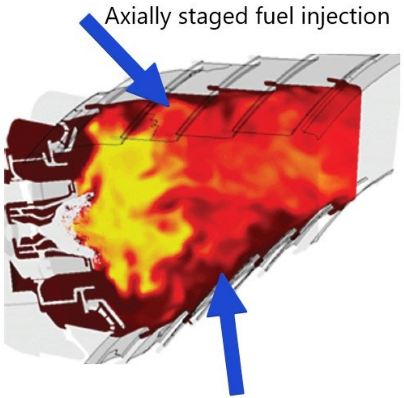
Reactor Network Modeling:

- GE and UCF will use Reactor network modeling to evaluate various combustor architectures.
- Fuel composition used will be based on results of Task 2.1 (Catalytic conversion of ammonia to hydrogen)



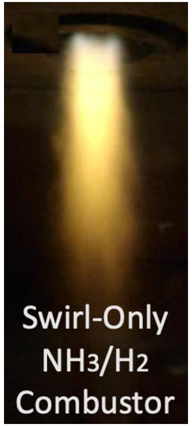
CFD with Validated Kinetic Model:

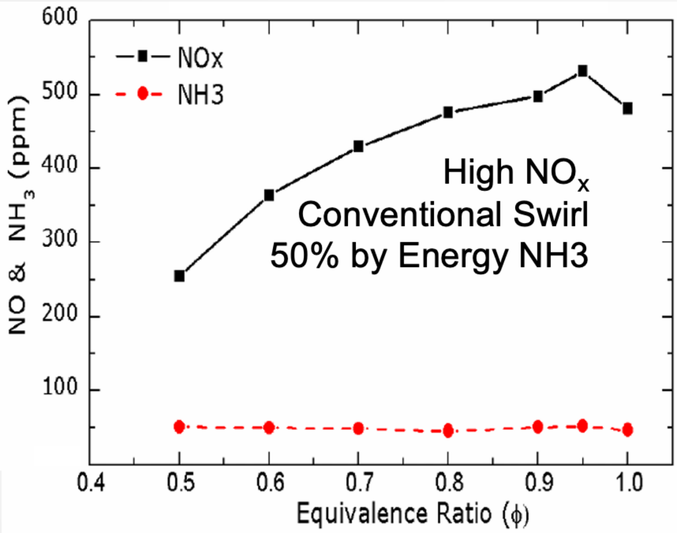
- CFD study using commercial CFD solver (Ansys/Star-CCM)
- Validated Kinetic model developed in subtask 2.2.2 (UCF) will be utilized.

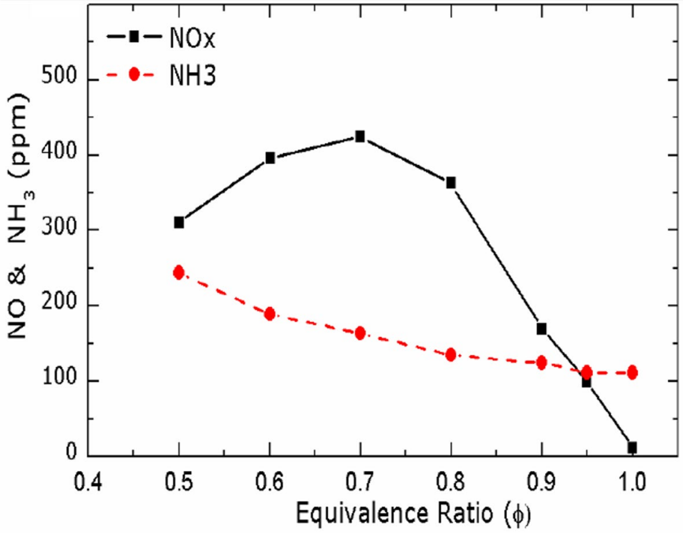


Purdue – Experimental Validation under Engine Representative Conditions

Challenge #1: Combustor Design Plays a Critical Role in NO_x and NH_3 in Exhaust



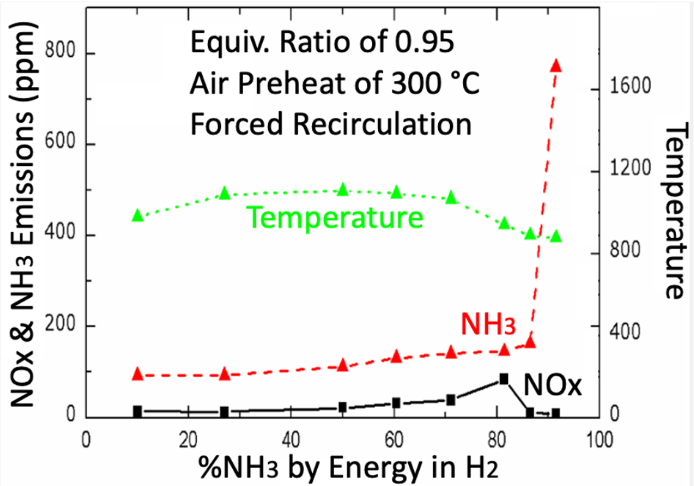




Meyer T, Kumar P, Li M. Ammonia combustion with near-zero pollutant emissions . NH3 Fuel Association; 2011. Available online https://nh3fuel.files.wordpress.com/2013/01/2011-meyer.pdf.

Purdue – Experimental Validation under Engine Representative Conditions

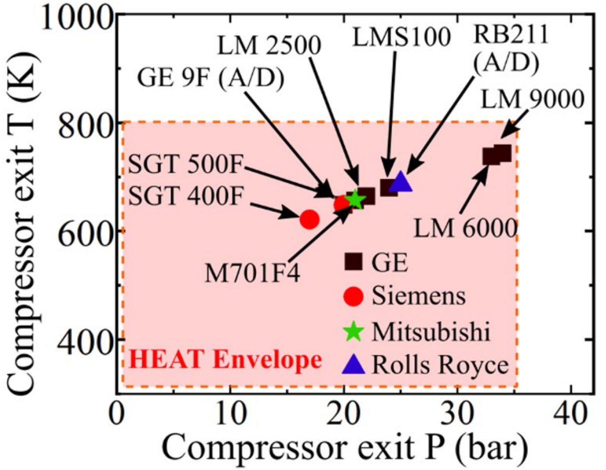
Challenge #2: NH_3 in Exhaust can Reform NO_x but the Risk is High NH_3 Slip



Meyer T, Kumar P, Li M. Ammonia combustion with near-zero pollutant emissions . NH3 Fuel Association; 2011. Available online https://nh3fuel.files.wordpress.com/2013/01/2011-meyer.pdf.

Challenge #3: Aviation Conditions

- High P, T and low residence times
- Extremely wide range of conditions
- Actual state of the fuel is not yet known



Aeroengine Conditions that can be Achieved in Purdue HEAT Rig (Compiled by Venkat Athmanathan, 2021)

GREATER ORLANDO AVIATION AUTHORITY SwRI Ansys GE BOEING PURDUE UNIVERSITY petal GT Georgia Tech Aerospace Systems Design Laboratory CATER UCF

Relevant Statistics from MCO Airport

Reports on Arrivals and Departures Data at MCO Airport Suggest Following Choices (flight counts are for year from SEP 01, 2021 to SEP 01, 2022):

(1) Aircraft: 737-900

Widely used,
but no longer in production

Most Common Route on United:
KMCO to KIAH (1379 flights)

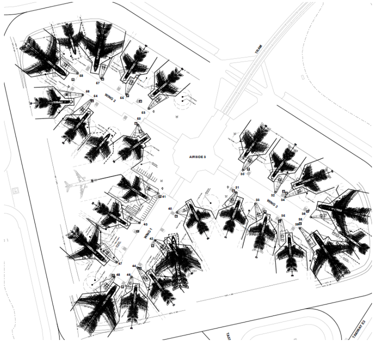
Engine: CFM 56-7B

(2) Aircraft: 737-8

In production

Most Common Route on United:
KEWR to MCO (534 flights)

Engine: LEAP 1B



United Airlines currently operates from 9 gates at Airside 3 at MCO, typically gates 40-48.

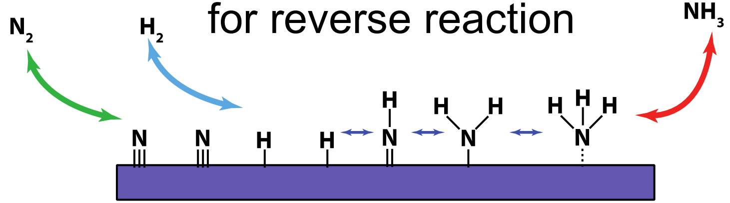
All gates at MCO are controlled by the Aviation Authority and can accommodate ADG III aircraft, which includes the Boeing 737.

The fuel pit/ hydrant locations will be made available to analysis teams for calculation of cost impacts.

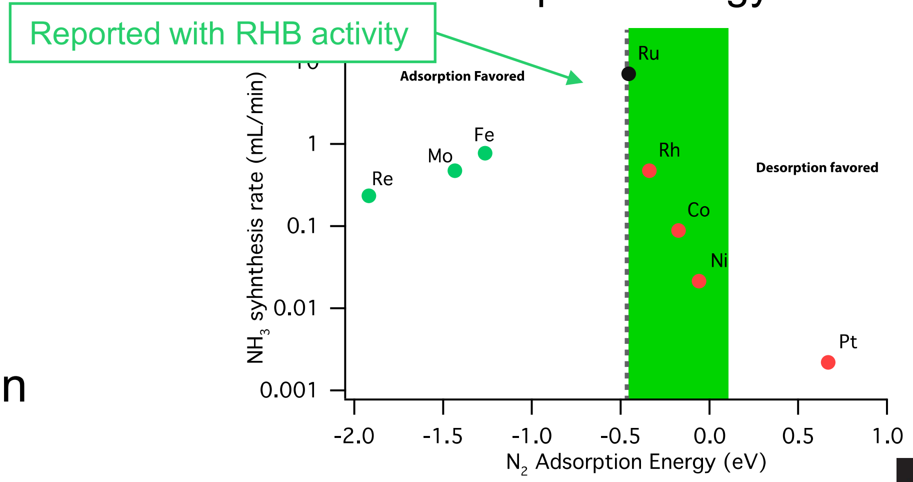
NH_3 Synthesis & Cracking

- $N_2 + 3H_2 \rightarrow 2NH_3$
  - Haber-Bosch Process
    - Entropically disfavored
    - High temperatures and pressures required
  - Iron and Ruthenium based catalyst
  - N_2 and H_2 must have favorable interaction with surface, but NH_3 desorption must be fast
- $2NH_3 \rightarrow N_2 + 3H_2$
  - Reverse Haber-Bosch (RHB) or catalytic cracking
  - NH_3 must have favorable interaction with surface, but N_2 and H_2 desorption must be fast

- Reversible Process – need to optimize for reverse reaction

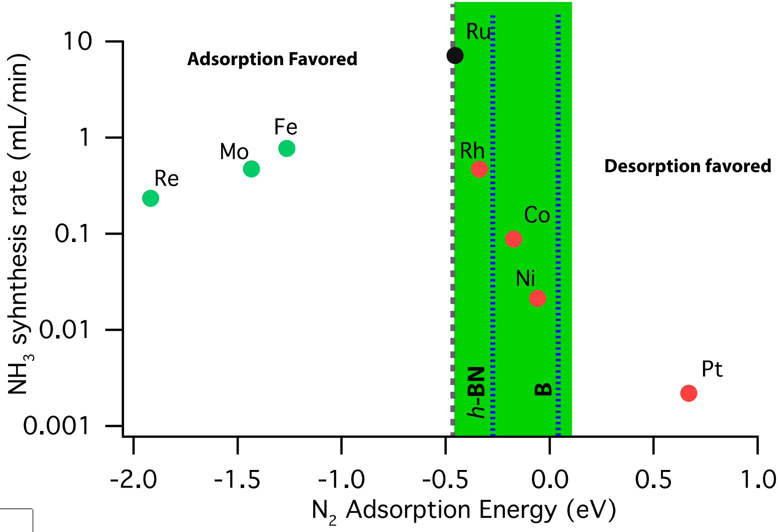


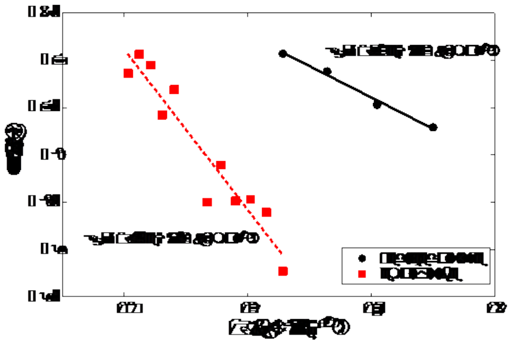
- Look at NH3 production rates vs. N2 adsorption energy



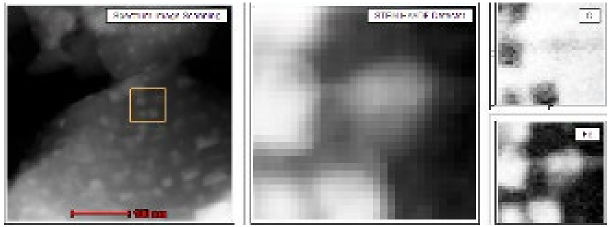
Improved Catalysts

- Most work focused on oxide and pure metals
  - Nitrides of interest but not yes implemented commercially.
- Nano-iron has activity
- Boron-based materials fall in sweet spot
  - Strong experience with boron-based catalysis
    - Hydrogenation, CO_2 reduction, hydrodenitrogenation



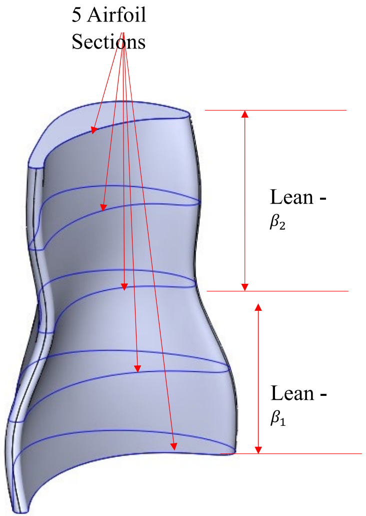


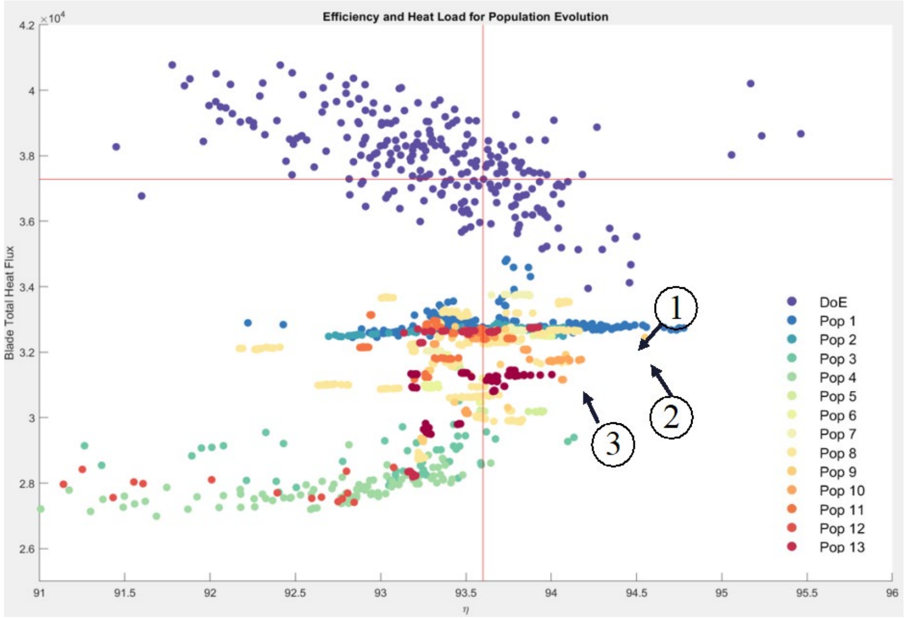
Active nano-iron from earth abundant mineral

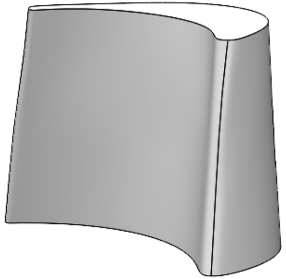


Optimization & Analysis of the Turbomachinery

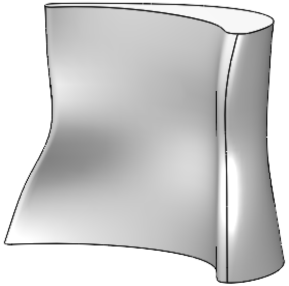
- Optimization based on genetic algorithms:







baseline



Joly, Verstraete, Paniagua, 2013, http://doi.org/10.1007/s00158-013-0987-5

Puente, Paniagua, Verstraete, 2015, https://doi.org/10.1016/j.apm.2014.07.003

sCO2 Waste Heat Recovery

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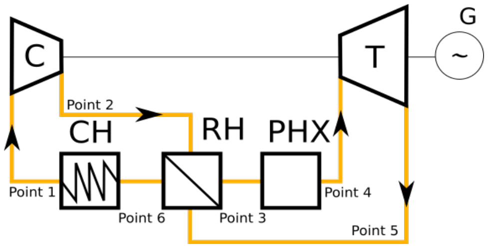
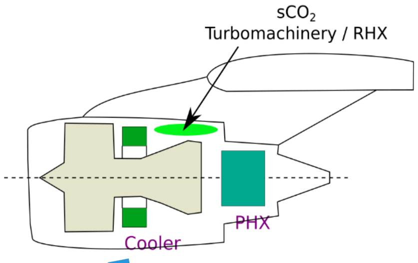
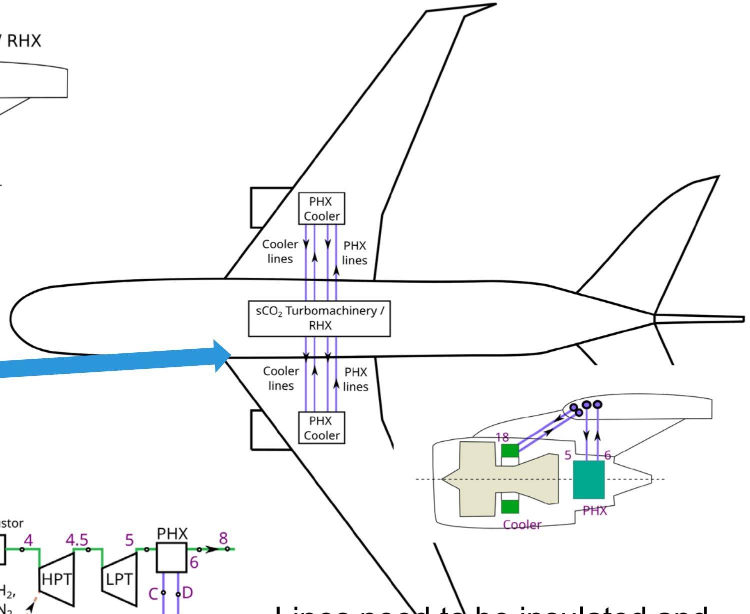
sCO2 Waste Heat Recovery (WHR) Cycle – System Integration

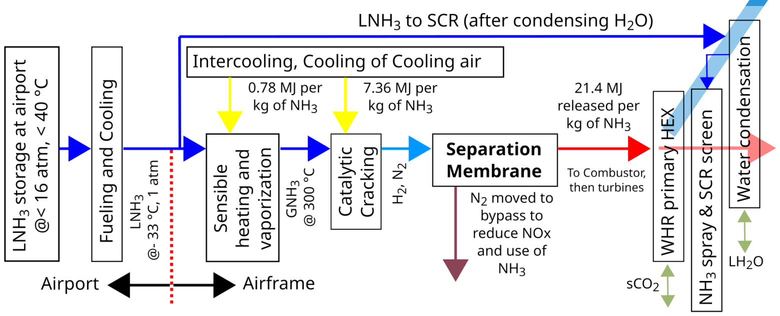


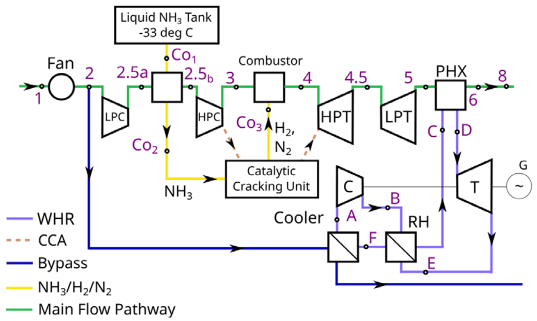




Potential Configurations

- Recuperated vs. non-recuperated
- Centralized (1 WHR per airplane) vs. distributed (1 WHR per engine)





Lines need to be insulated and overall wing construction must be re-designed to prevent possible damage due to line malfunction.

System Modeling & System Impact

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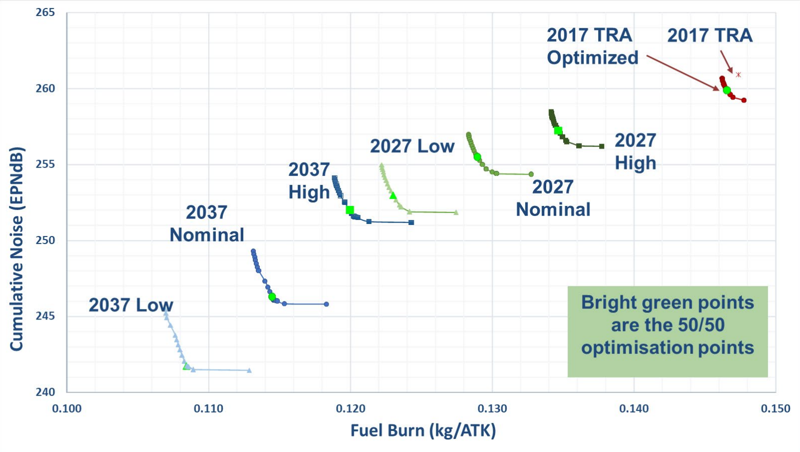
Recent Relevant Activities (from ASDL)

Previous/Ongoing Studies

- IEIR Study:
  - Independent industry experts engaged in reviewing GT modeling to project vehicle classes to the 2037 time frame
- Long Term Aspirational Goals for CAEP (LTAG):
  - One of three key legs of future aviation goal setting (fuels, operations, and technology)
  - *Dr. Mavris* is the co-lead for aircraft technology
- Electric Propulsion Flight Demonstrator (EPFD) Systems Analysis of Advanced Concepts:
  - To understand potential benefit of proposed vision systems relative to established program goals
- Continuous Lower Energy, Emissions, and Noise (CLEEN) System Level Assessment:
  - Technology and vehicle modeling to understand long term impacts of novel technologies to US fleet
- NASA Environmentally Responsible Aviation (ERA)
- NASA ULI: OSU and IZEA



Common analysis framework developed

- Starting point vehicles in our analysis (B737-8)
- Common framework for analyzing all of the concepts


Boeing 737-8


Boeing Transonic Wing Concept

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Transient System Modeling with T-Mats and IDAES

IDAES (Institute for the Design of Advanced Energy Systems) model.

The open-source software

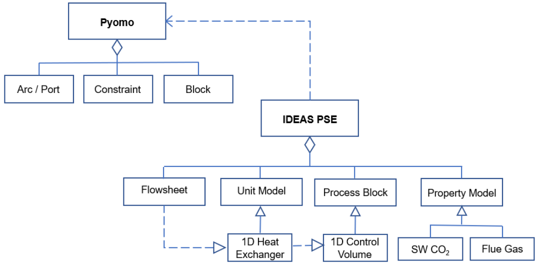
Capabilities: -- static and dynamic simulation of

- full range of advanced fossil energy systems
- chemical looping and other transformational CO_2 capture technologies
- supercritical CO_2 Power systems.

IDAES
Institute for the Design of Advanced Energy Systems

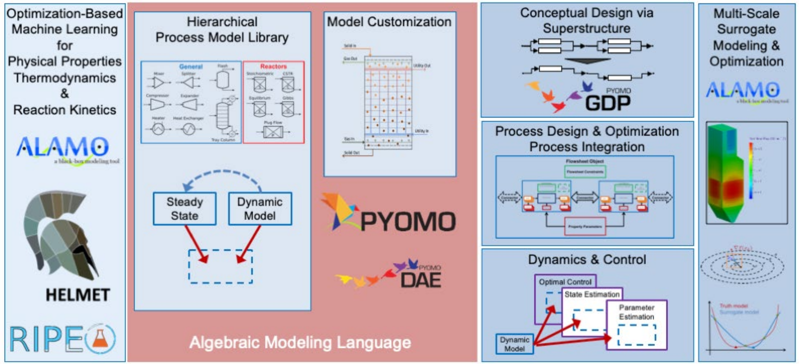
https://idaes.org/

Ideas architecture:



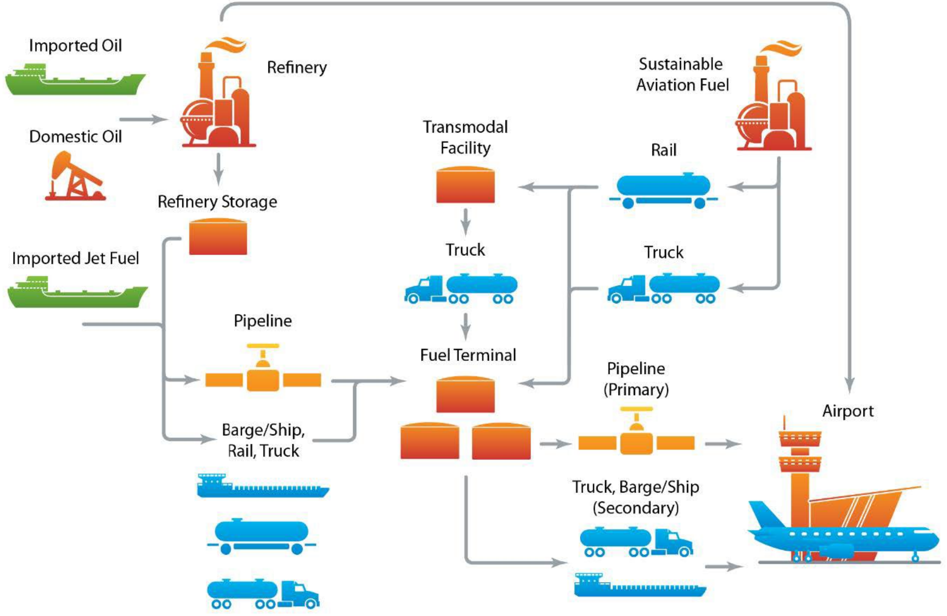
The IDAES framework can be used for:

- process synthesis and conceptual design, including process intensification,
- process design and optimization, including process integration,
- process control and dynamic optimization,
- using advanced solvers and computer architectures,
- automated development of thermodynamic, physical property, and kinetic submodels from experimental data,
- integration of multi-scale models,
- comprehensive, end-to-end uncertainty quantification, including stochastic optimization,
- maintaining complete provenance information, and
- the ability to support multiple scales, from materials to process to market.



Assessment of Airport Ground Infrastructure

- Work with stakeholders to examine airport infrastructure
  - Use literature for broad assessment
  - Work with an airport partner to examine specific needs
  - Author preliminary plan for infrastructure changes
- Compare against other projections of sustainable fuel upgrades
  - Sustainable aviation fuel (SAFs)
  - Hydrogen, liquid or gaseous



Source: Moriarty and Kvien, “U.S. Airport Infrastructure and Sustainable Aviation Fuel”, *National Renewable Energy Laboratory,* Report NREL/TP-5400-78368, February 2021

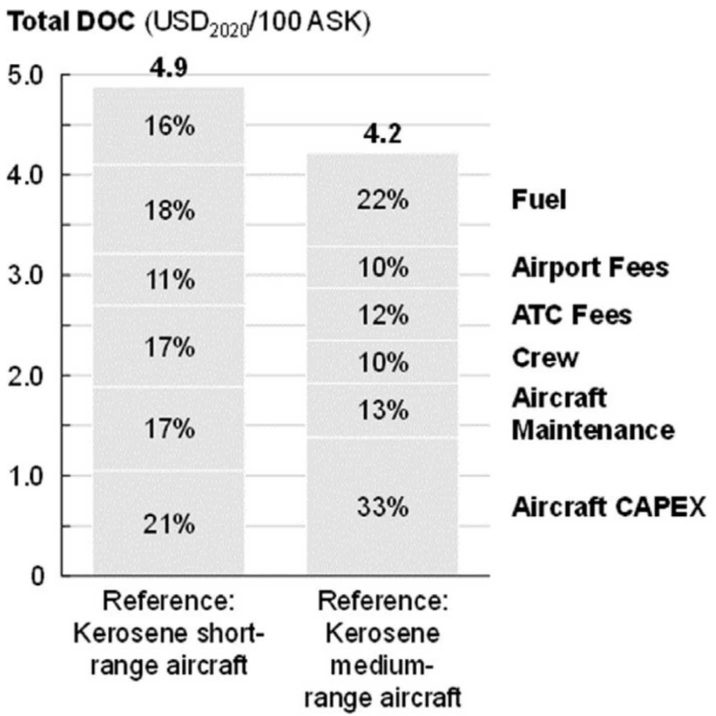
Hazard & Risk Analysis

- Industrial safety practices
  - Government and private best practices
  - Appropriate regulatory documentation
  - Identification of pain points
- Handling strategy
- Risk mitigation
- Creating new standards

- Regulated
- Flammable
- IDLH at 300 ppm
- Corrosive
- Cryogen
- Water soluble
- Theft
  - Drugs
  - Explosives

Order of Magnitude Cost for Airport Upgrade

- Develop preliminary installation cost
  - Major equipment
  - System changes and upgrades
- Use in-depth analysis of a single gate to estimate airport-wide cost
- Develop operating cost impacts
  - Compare against other proposed sustainable fuels
  - Use normalizing metrics such as dollars per available seat kilometers



Source: Hoelzen, et al., "Hydrogen-powered aviation and its reliance on green hydrogen infrastructure – Review and research gaps", *International Journal of Hydrogen Energy Volume 47*, Issue 5, 15 January 2022, Pages 3108-3130

Modeling Roadmap to understand this complex System of Systems

- MTOW
- Startup / Shutdown
- Operational viability
- $ / passenger-mile

Engine

- Intercooling
- Cooled Cooling Air
- Combustion

→ Changes in SFC

Airframe

Engine Integration

- Cracking
- Water Condensation
- Selective Catalytic Reduction

→ Size, Mass, Power

NH3/NOx/H2O System

sCO2 WHR

- System Model
- Turbomachinery
- Heat Exchangers
- Electrical
- Layout

→ Size, Mass, Power

→ System Models will inform Component Designs, and vice versa

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Technology Transition & Demonstration

Technology Transition & Demonstration

Potential Ground Demonstration of selected components on J85 Engines, in partnership with Larsen Motorsports, @ Valkaria Airport. Larsen Motorsports participates in this project through Peer Review Board.

Technology Maturation of Components

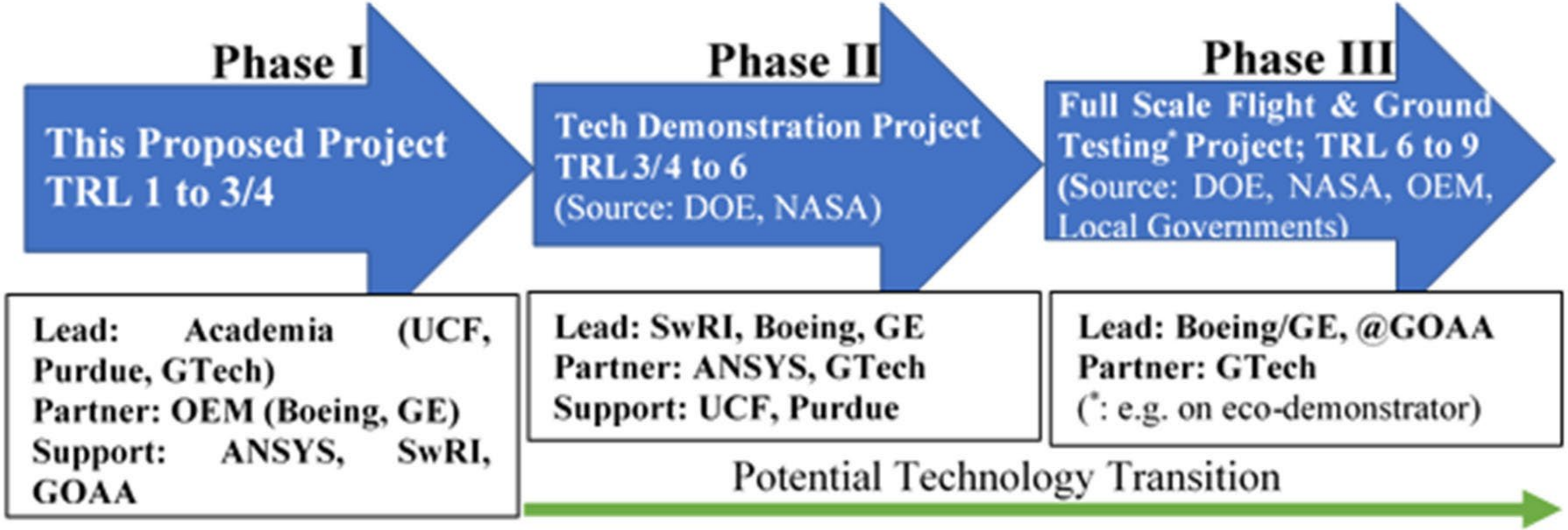
Optimization of integrated Systems

Ground demonstration

Flight Demonstration

Boeing's Broad Interest in this Project Should Lead to Flight Demonstration Opportunities

Technology Transition Plans



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Thank you for your Attention!

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Heavier-than-air flying machines are impossible.
Lord Kelvin, 1895

It is apparent to me that the possibilities of the aeroplane,
. . . have been exhausted, and that we must turn elsewhere.
Thomas Edison, 1895

Flight by machines heavier than air is unpractical and insignificant, if not utterly impossible.
Simon Newcomb, 1902

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