UTSR AND ADVANCED TURBINES PROJECT REVIEW MEETING 2023

AMMONIA FUEL PRECONDITIONER FOR GAS TURBINES

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ACKNOWLEDGEMENTS

DOE-FECM

- Purdue University, “Investigation of Flame Structure for Hydrogen Gas Turbine Combustion,” UTSR Project FE0032074
- Argonne national Laboratory, “Ammonia fuel preconditioner for gas turbines,” FWP 38668.1
- Generous support of the computing resources by Laboratory Computing Resource Center (LCRC) at Argonne National Laboratory

POSITIVES

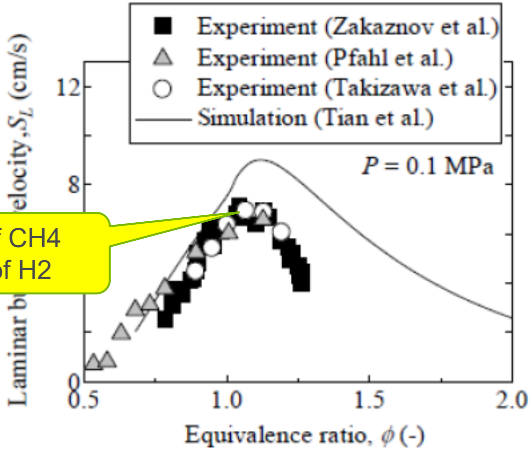
- Well developed NH_3 synthesis process
  - Haber-Bosch process
- Easy storage & transportation
  - 8 bar, 20°C, liquid
- High Hydrogen content
  - 17.7 wt%, 108 gH_2/Liter
- No carbon emissions

NEGATIVES

- Toxic!!!
  - But is used extensively for agricultural purposes
- High NO_x emissions
  - 200 to 2000 ppmv typical
- N_2O emissions
  - Has GWP of 273
- NH_3 slip in exhaust

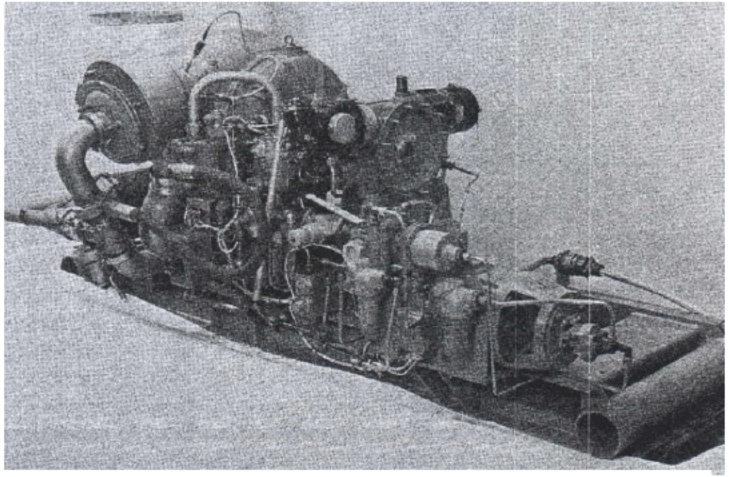
and…

NH_3-AIR MIXTURES HAVE EXTREMELY LOW FLAME SPEEDS



1/2X that of CH4
1/6X that of H2

S_L of NH_3-air laminar premixed flame (Hayakawa,2015)



Solar model T-350 engine (Solar, *Final Technical Report*, DA-44-009-AMC-824, 1968)

- NH_3-air combustion is difficult because the laminar burning velocity is much lower than that of conventional hydrocarbon fuels.
- In 1967, Pratt examined an NH_3-fired gas-turbine combustor, and concluded that combustion efficiencies were unacceptably low.
- Verkamp showed that the pre-cracking of NH_3 and the additives improved the flame stability
- Because of those difficulties, the research and development of NH_3-fueled gas turbines were abandoned, and it has not been retried until recently.

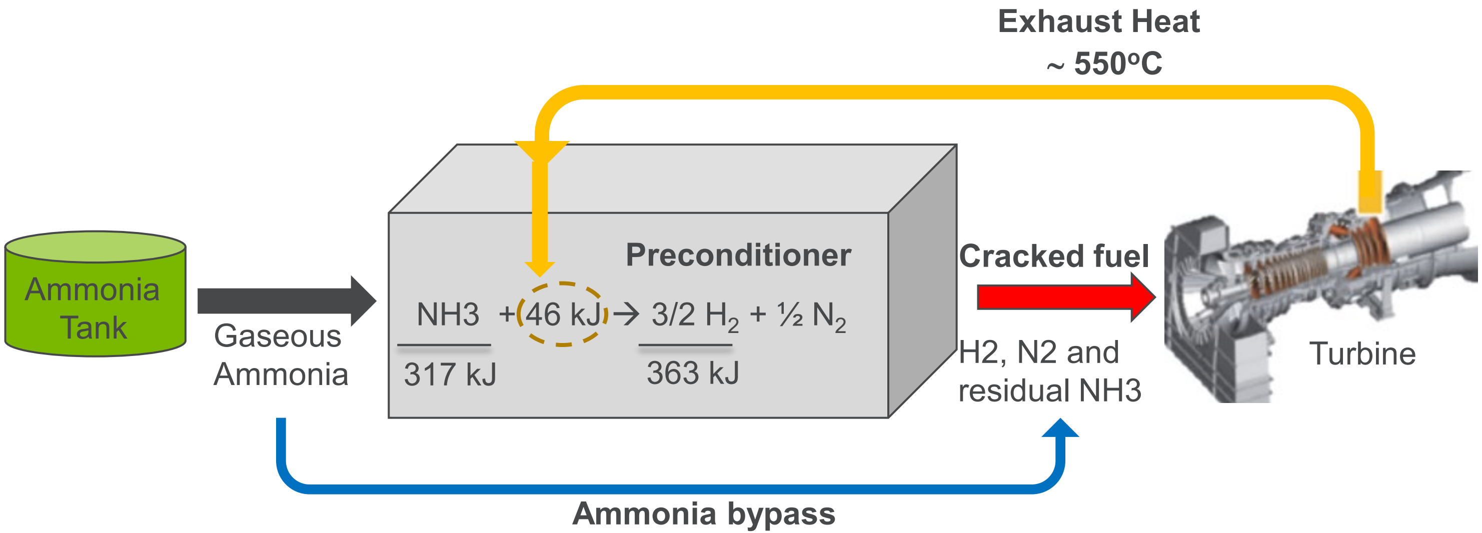
OUR GOAL

Design and develop a scalable, low-cost, low-power, fuel preconditioning system that enables use of Ammonia in stationary gas turbines with minimal changes to turbine hardware.

Implied targets

- Efficiency ~ 40% simple cycle
- $NO_x < 15$ ppv (15% O_2)
- Acceptable combustion stability

FUEL PRECONDITIONING SYSTEM



Exhaust Heat
~ 550°C

Ammonia Tank

Gaseous Ammonia

Preconditioner

$NH3 + 46\ kJ \rightarrow 3/2\ H_2 + ½\ N_2$

317 kJ

363 kJ

Cracked fuel

H2, N2 and residual NH3

Turbine

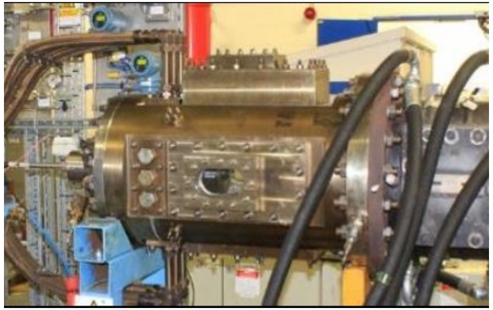
Ammonia bypass

Aim is to have minimal/no changes to combustion hardware

Year-1

Year-2

Year-3



Phase1: Low-T Dissociation Strategy
- Low-T catalyst

Phase2: COMBUSTOR SYS. DEV.
- CFD Study

Phase3: Fuel Preconditioner design & build

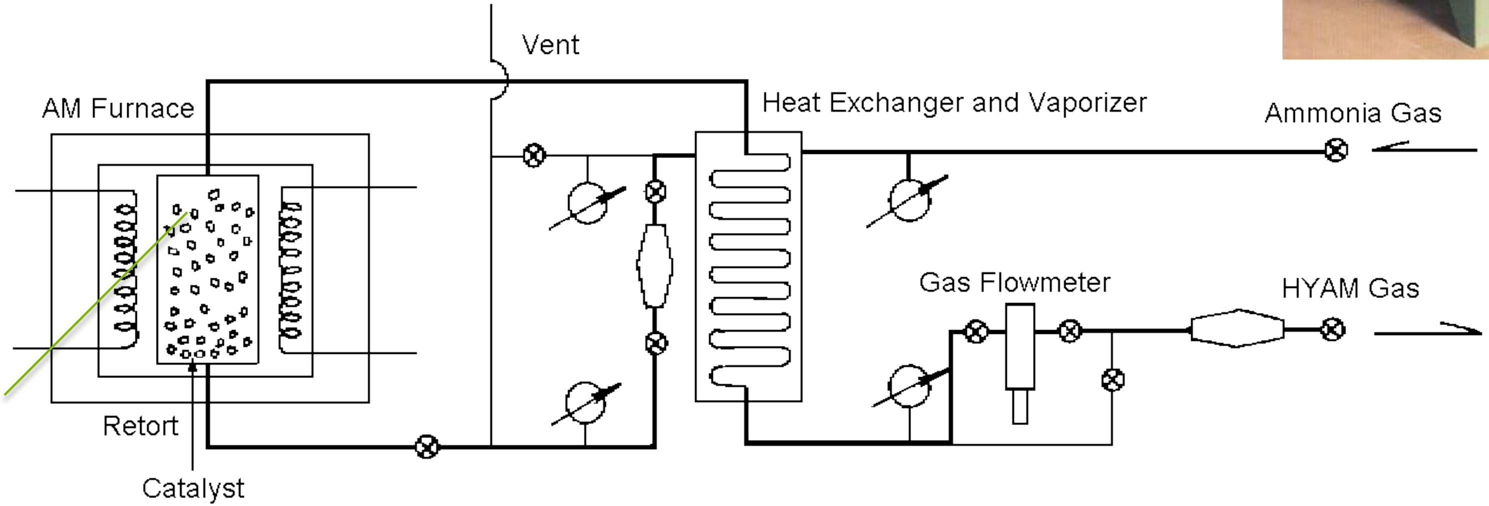
Phase4: Demonstration in 1MW Combustor
- Fueling infrastructure
- Testbed prep.
- Demonstration tests

PHASE-1: LOW-T DISSOCIATION STRATEGY

- LOW-T CATALYST

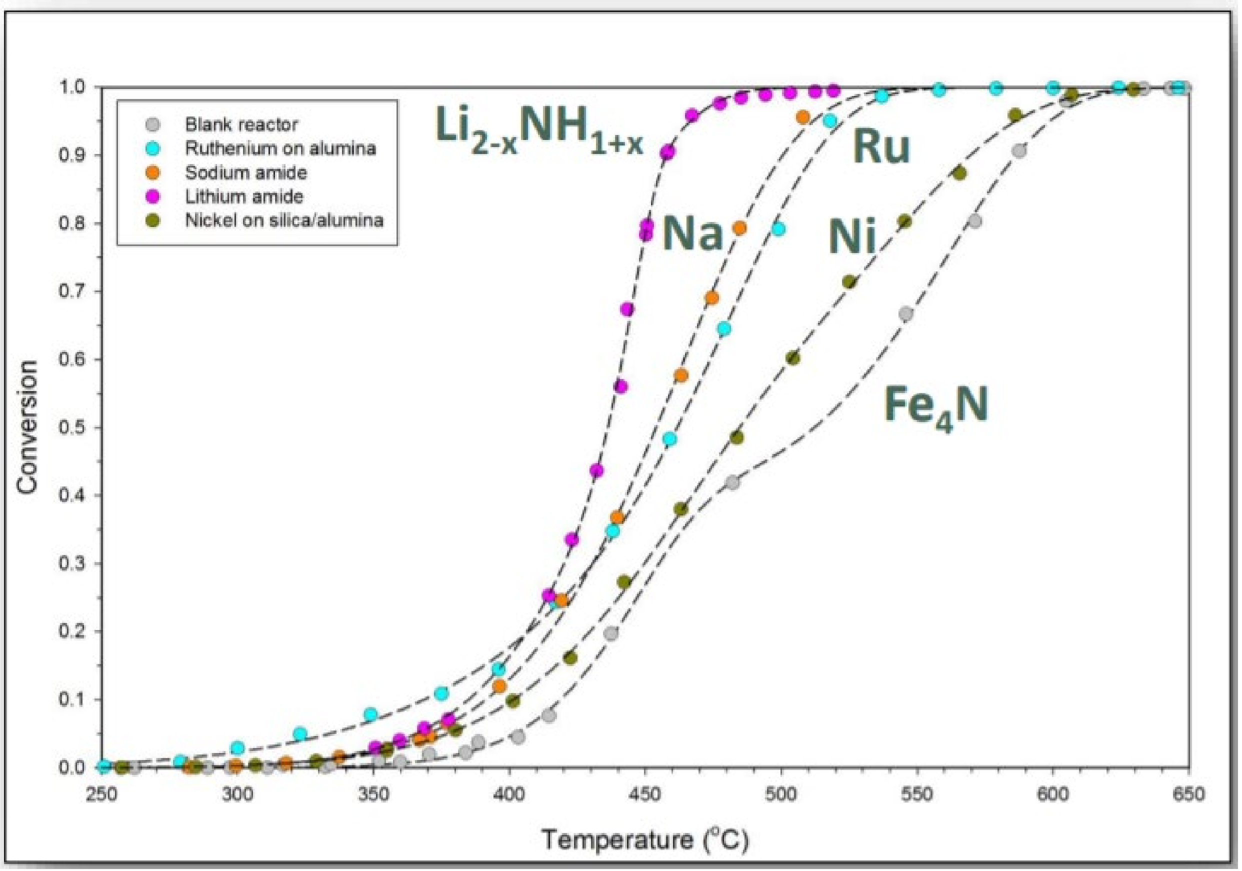
A TRADITIONAL AMMONIA CRACKER

Mainly used for metal heat treating applications



T ~ 850-950^{o}C

LOW-TEMPERATURE, COST-EFFECTIVE, DURABLE CATALYST

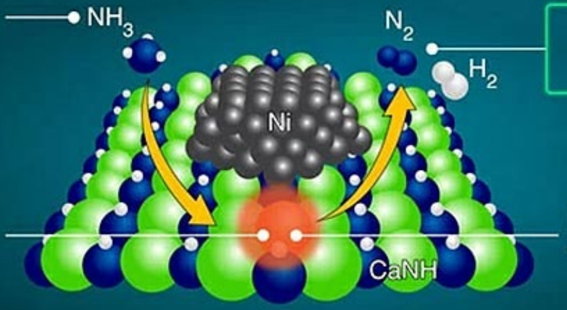


Producing Hydrogen from Ammonia Using State-Of-The-Art Calcium-Supported Nickel Catalyst

Nickel (Ni) catalysts decompose ammonia (NH_3) into nitrogen (N_2) and hydrogen (H_2)

- Require high temperatures
- Have low conversion activity

Novel Ni catalyst on calcium imide (CaNH) support



NH_3 absorbed on catalyst surface

N_2 and H_2 production

Activation by NH_2-vacancy site (V_{NH})

Regeneration of V_{NH}

- High conversion activity
- High durability
- Low operating temperature

Ni-supported CaNH is a durable and highly active catalyst for efficient H_2 production from NH_3

Ammonia Decomposition over CaNH-Supported Ni Catalysts via an NH^{2-}-Vacancy-Mediated Mars–van Krevelen Mechanism

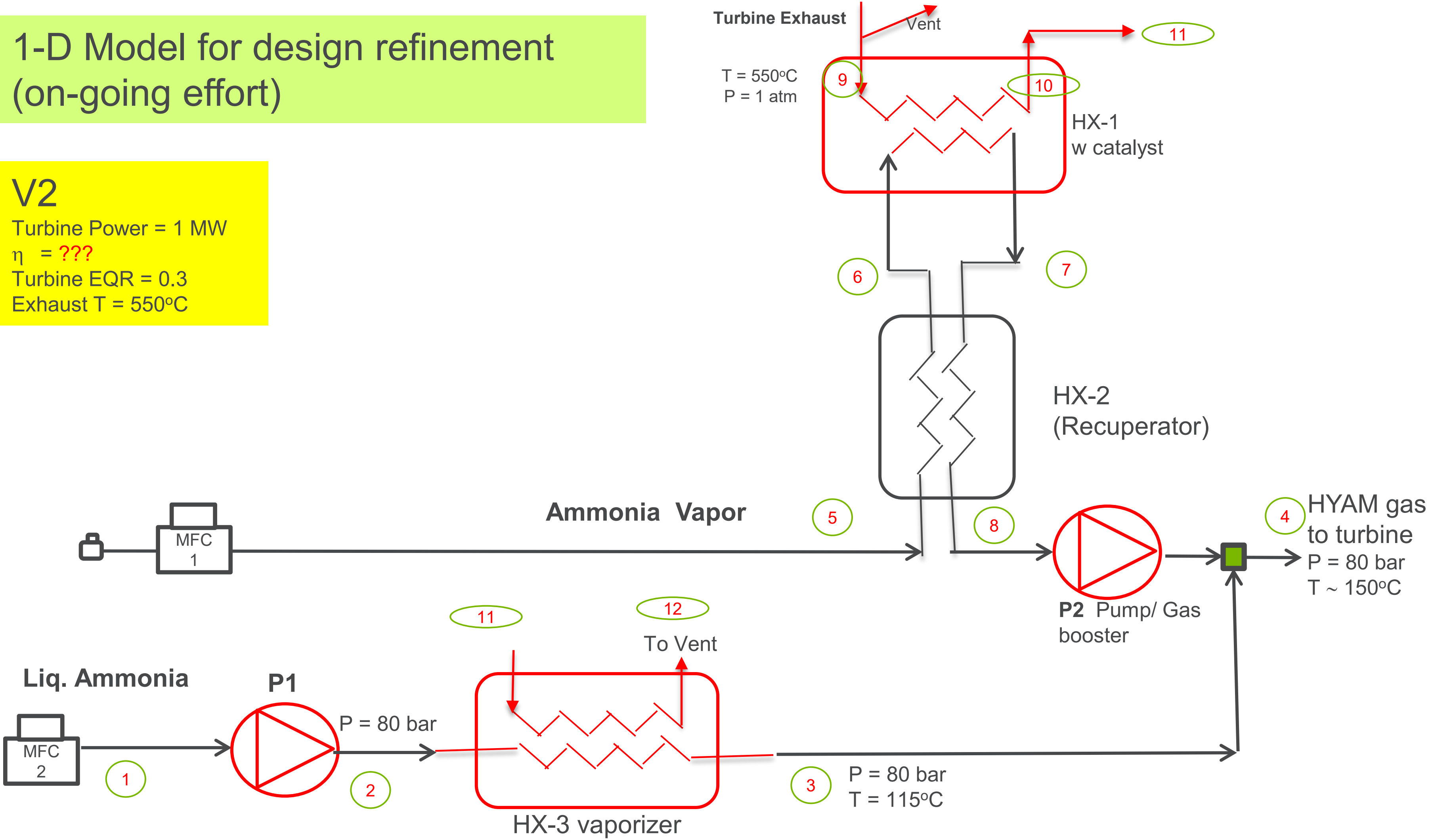
Ogasawara *et al.* (2021) | 10.1021/acscatal.1c01934 | *ACS Catalysis*

東京工業大学
Tokyo Institute of Technology

1-D Model for design refinement (on-going effort)

V2

Turbine Power = 1 MW
η = ???
Turbine EQR = 0.3
Exhaust T = 550°C



PHASE-2: COMBUSTION SYSTEM DEV.

- CFD

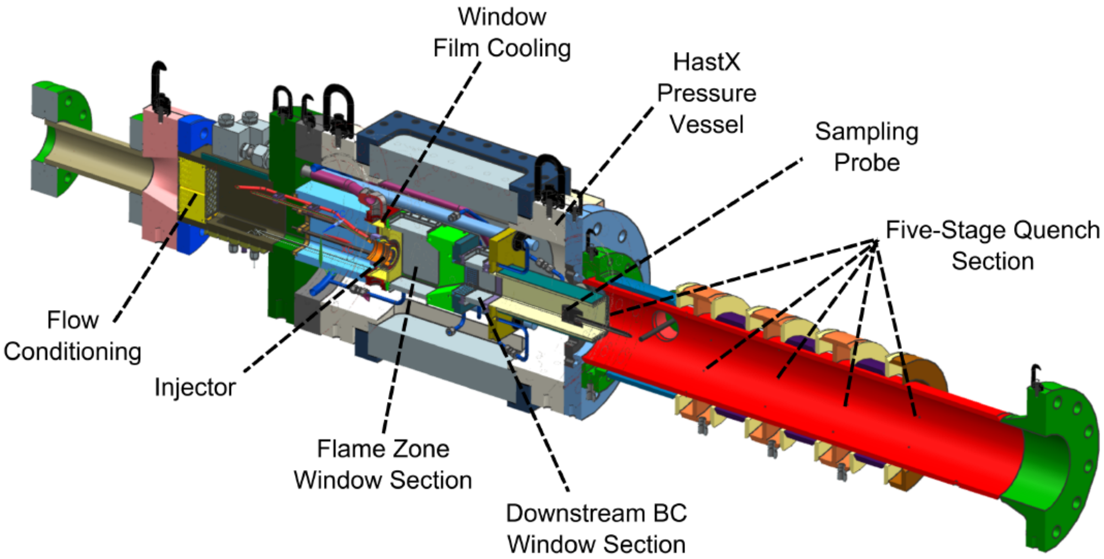
PURDUE'S COMRAD COMBUSTOR IS BEING USED AS THE TEST PLATFORM

Purdue's COMRAD Combustor

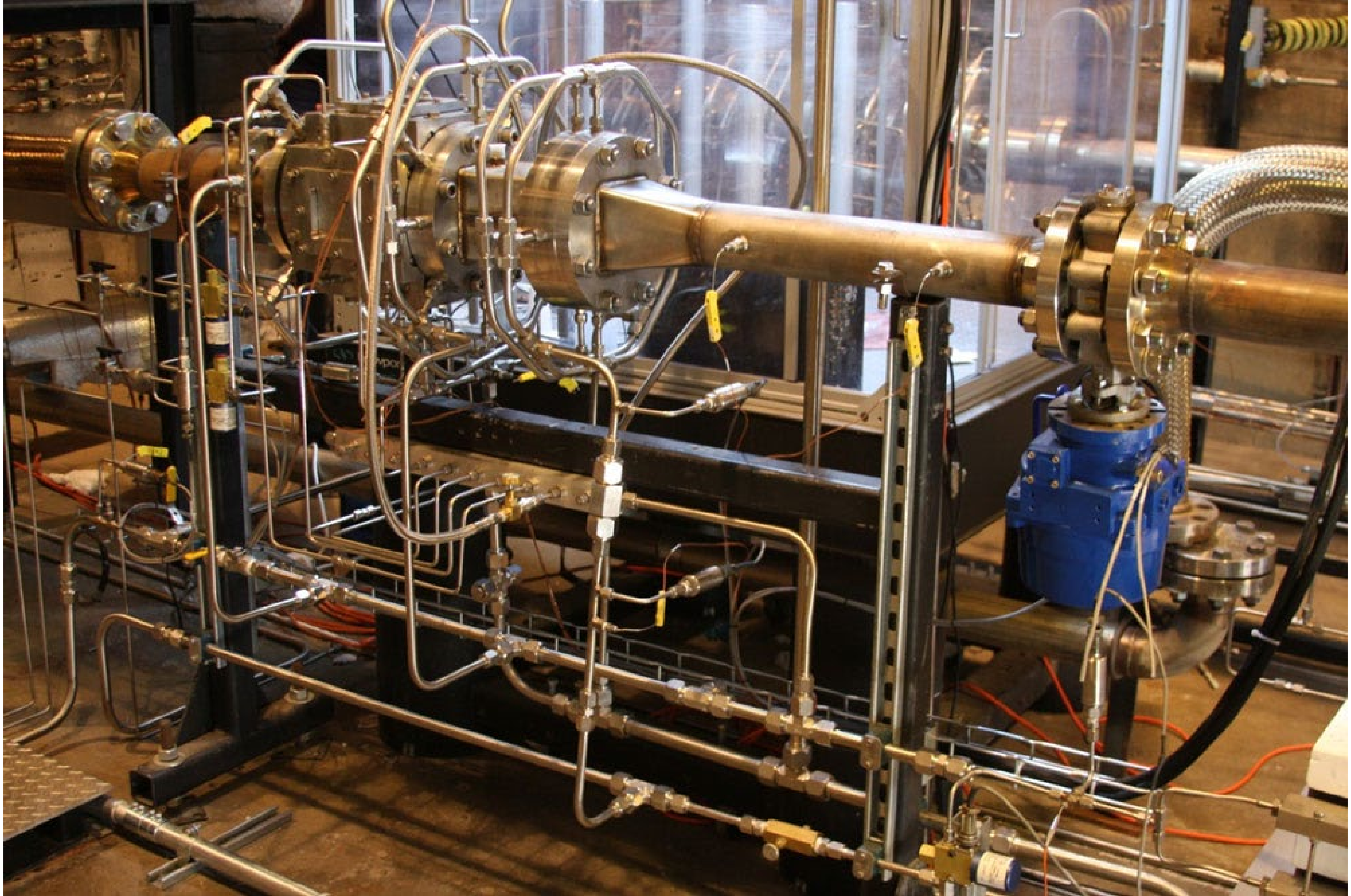
Max. P_3 = 40 bar
Max. T_3 = 760^{o}C
Max. Air flow = 3.6 kg/s
Thermal power density ~15 MW/m^2/bar)
Water cooled test article

Gas cooled windows

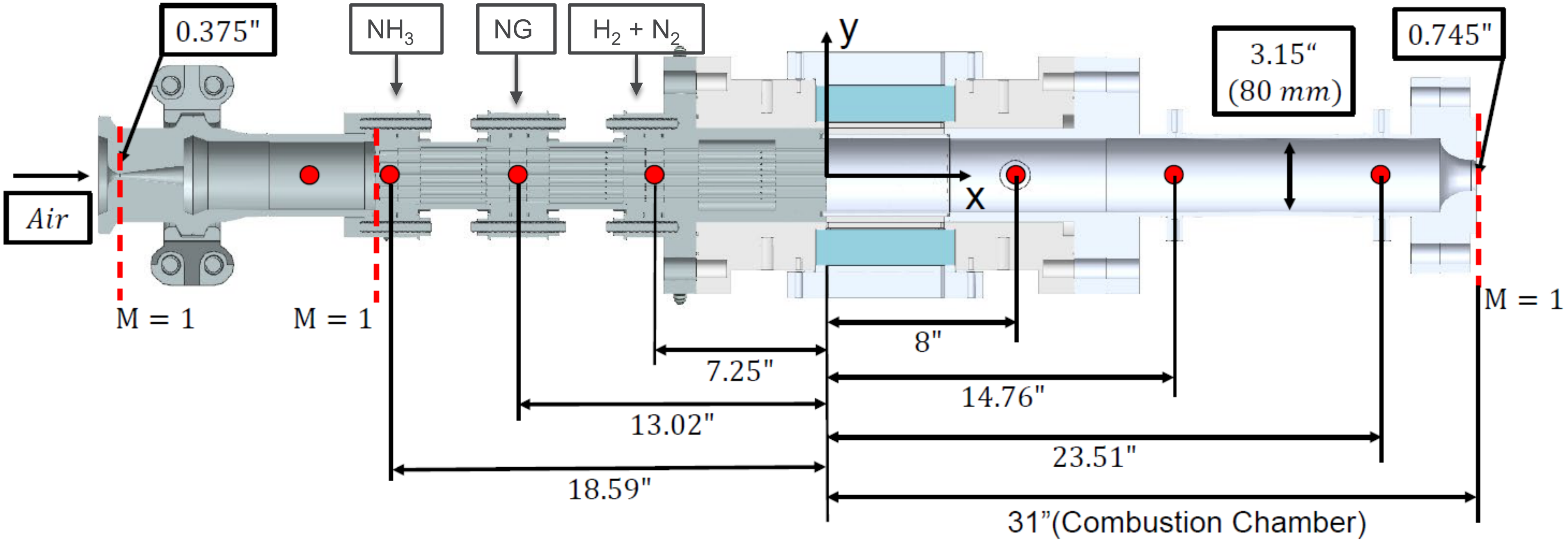
A variety of test instrumentation



Purdue 1 MW combustor

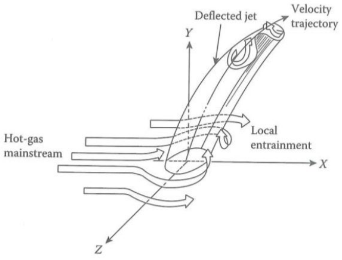


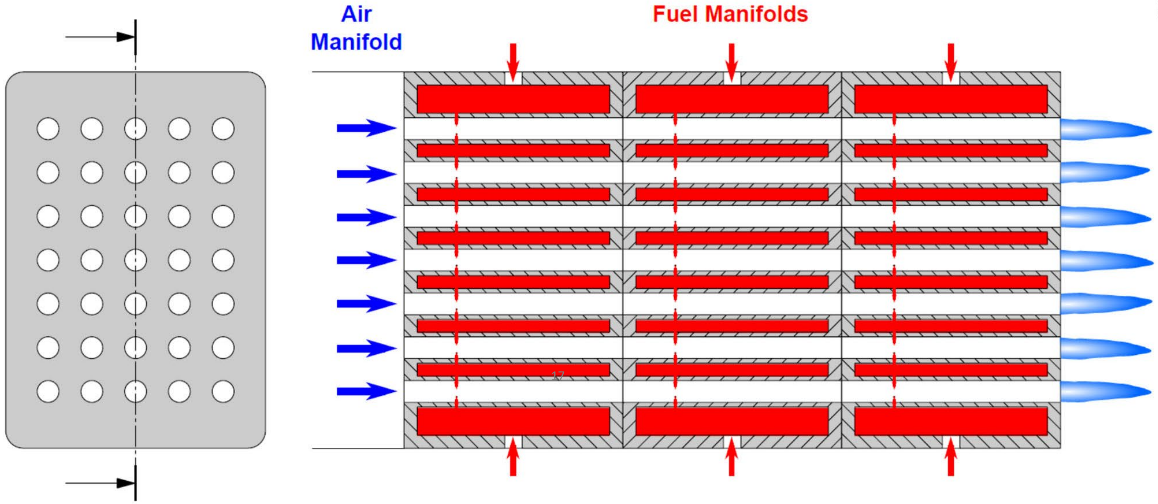
● Kulite WCT12M-35/70BARA 1 MHz Sampling



Argonne NATIONAL LABORATORY

MULTI-STAGE, MULTI-TUBE MICROMIXING (M^3) INJECTOR



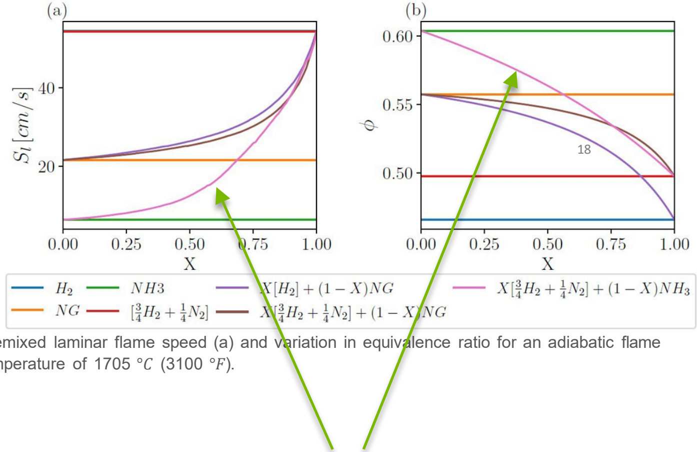


Schematic representation of the M^3 injector

EXPERIMENTAL & COMPUTATIONAL TEST MATRIX

- Initial fuel fraction (X) sweep from 0.5 to 1.0
- Ammonia decomposition efficiency (η) sweep from 0.4 to 1.0
  - ○ Rate of ignition delay increase requires unreasonable combustor lengths at $\eta < 0.4$
- Equivalence ratio determined at a fixed adiabatic flame temperature of 1980 K (DOE target for 65% combined cycle efficiency GTs)

$$X\left[\eta\left(\frac{3}{2}H_2+\frac{1}{2}N_2\right)+(1-\eta)NH_3\right]+(1-X)NG$$



Premixed laminar flame speed (a) and variation in equivalence ratio for an adiabatic flame temperature of 1705 °C (3100 °F).

Our interest

Fluid	X	η	$\dot{m}_{max}$ $[kg/s]$	$P_{bulk,min}$ $[bar$
H_2	1.0	1.0	0.03	55
N_2	1.0	1.0	0.13	47
NG	0.0	N/A	0.04	47
NH_3	1.0	0.4	0.09	N/A
Air	N/A	N/A	2.2	62

CFD EVALUATIONS

All simulations were performed using CRUNCH-CFD by CRAFT-Tech.

- **Task-1**

  Non-reacting flow evaluation of micromixing arrangement
  - NH_3 crossjet in air
  - H_2/N_2 crossjet in air

- **Task-2**

  (Natural Gas – air) reacting flows for experimental validation

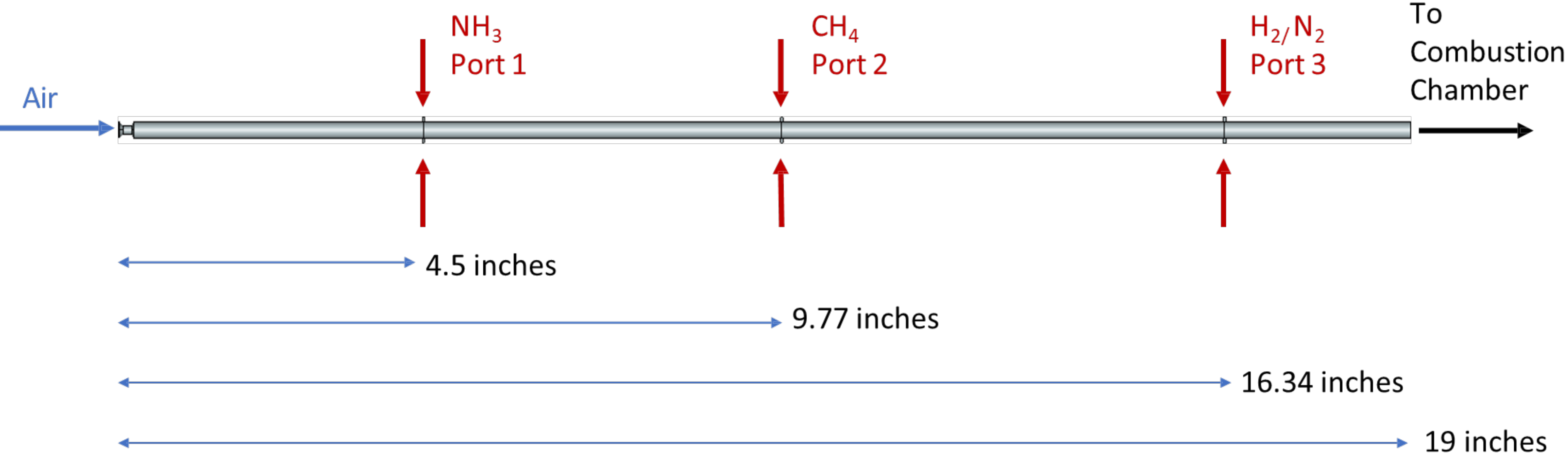
- **Task-3**

  (NH_3 – H_2/N_2 – air) reacting flows

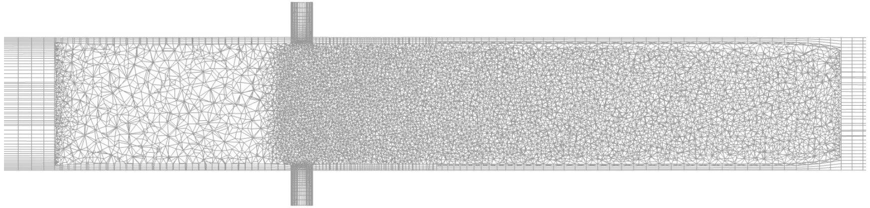
			Task 1		Task 2	Task 3		
			Case1	Case2	Natural Gas	Ammonia1	Ammonia2	Ammonia3
	Fuel Composition		100% NH3	100% H2	NG/H2/N2 mix	NH3/H2/N2 mix	NH3/H2/N2 mix	NH3/H2/N2 mix
NH3 @ 305.4K	Fuel Inlet Mass Flow1	kg/s	0.00207	0	0	0.023638	0.01970	0.01576
NG @ 294.3K	Fuel Inlet Mass Flow2	kg/s	0	0	0.010	0	0	0
H2 @ 294.3K	Fuel Inlet Mass Flow3	kg/s	0	0.00037	0.002	0.00280	0.00350	0.00420
N2 @ 294.3K	Fuel Inlet Mass Flow4	kg/s	0	0.00171	0.008	0.01296	0.01620	0.01944
	Oxidizer Inlet Mass Flow	kg/s	0.0239	0.0239	0.454	0.454	0.454	0.454
	Oxidizer Inlet Temp.	K	755.4	755.4	755.4	755.4	755.4	755.4
	Exit Back Pressure	MPa	1.034	1.034	1.034	1.034	1.034	1.034

TASK-1: NONREACTING FLOW MICROMIXING

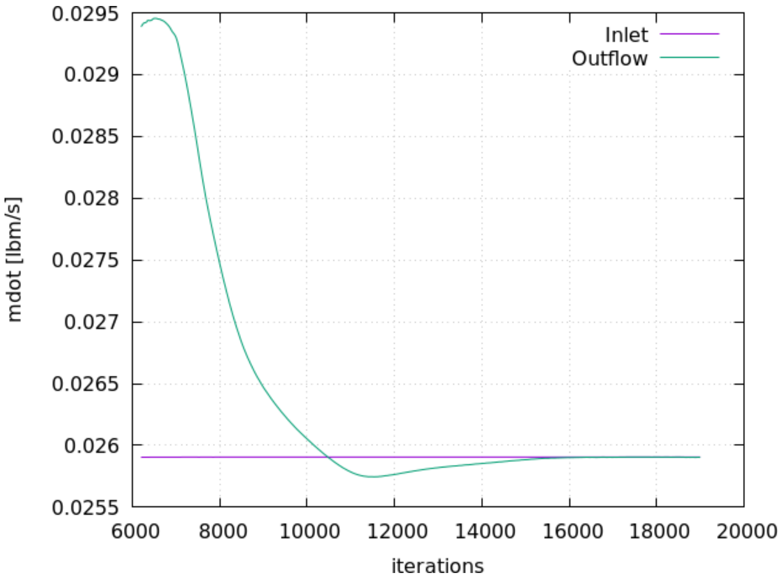
- Geometry: a single injector tube
- Steady state RANS cold flow (non-reacting) simulation calculations:
  1. Case 1: Pure NH_3 with air
  2. Case 2: H_2/N_2 mixture with air



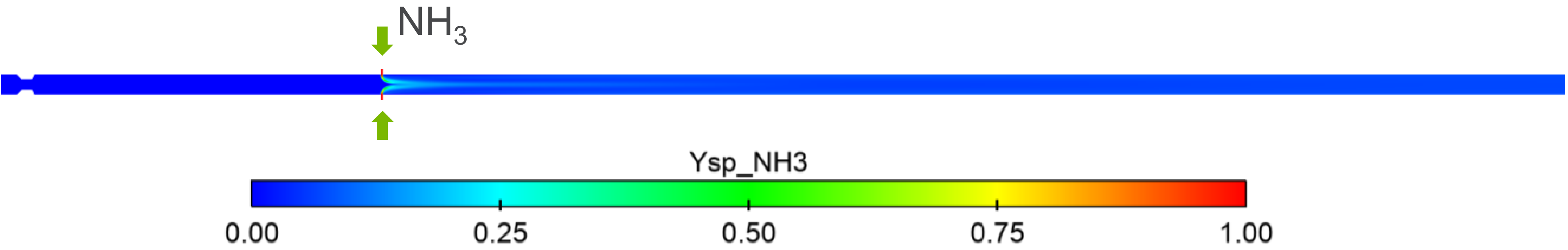
TASK-1 SIMULATION OVERVIEW

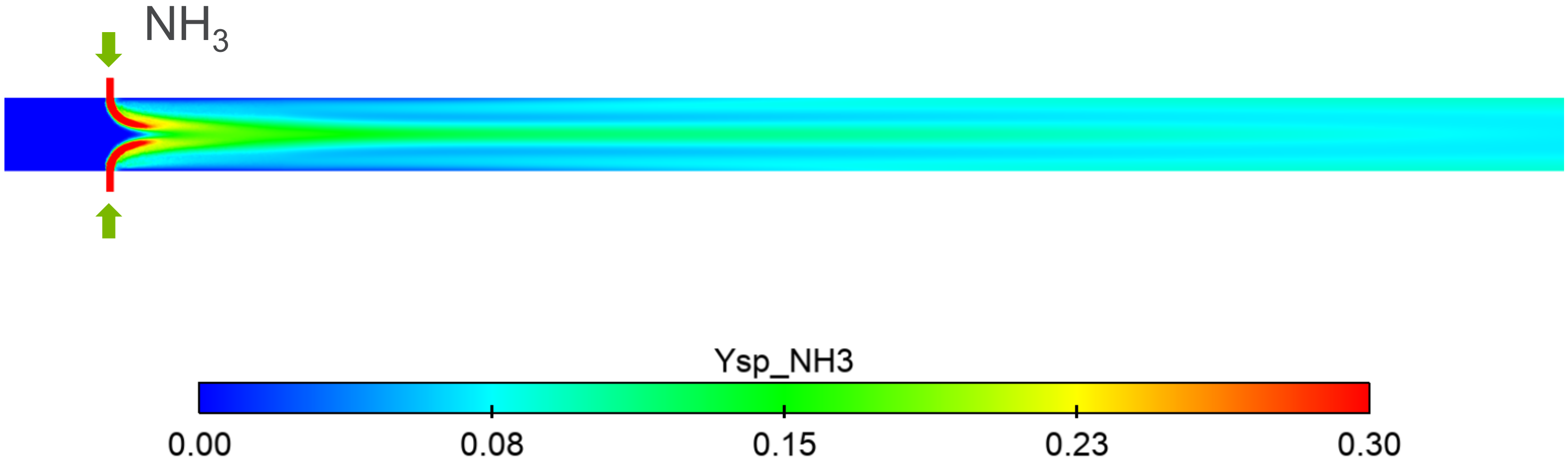


- Inputs:
  - Non-reacting multi component simulation
  - Steady-state
  - k-ε turbulence model with wall function
- Grid:
  - Hybrid unstructured mesh
  - ~900,000 cells
  - Significant resolution required near injection ports
  - Multiple grid iterations were required to accurately resolve jet and obtain good mass flow convergence

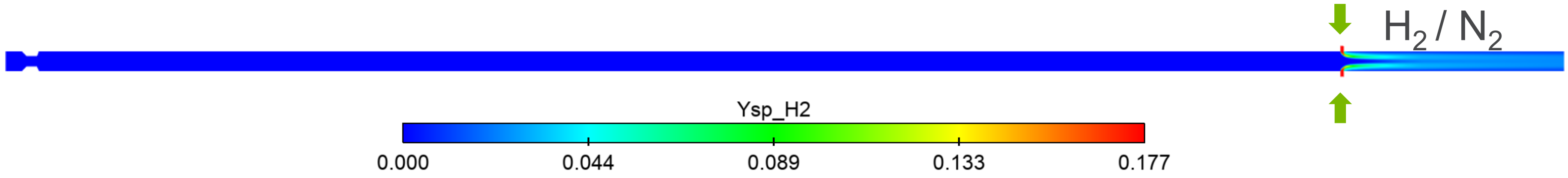


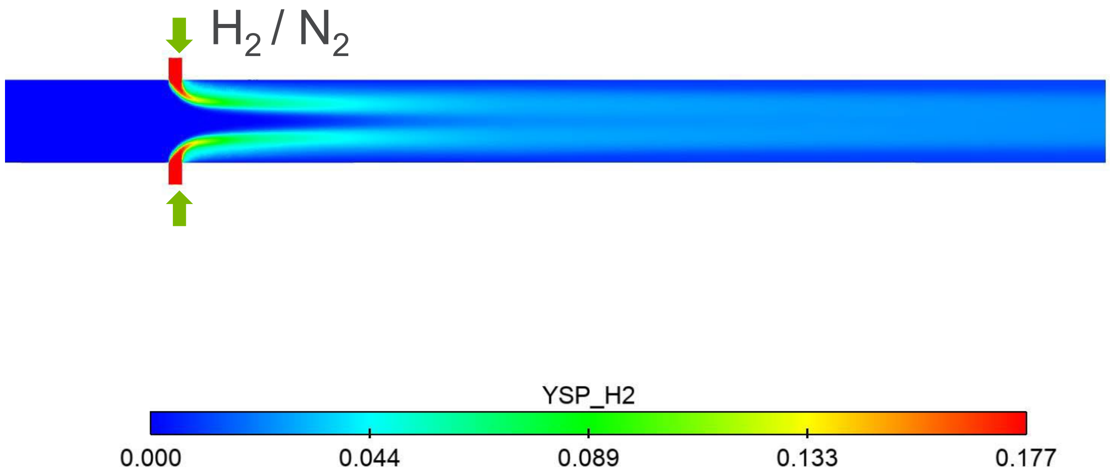
TASK-1: NH3 INJECTION





TASK-1: H_2/ N_2 INJECTION





TASK-2: COMBUSTING SIMULATIONS OF (NG/H_2 /N_2) MIXTURE IN AIR

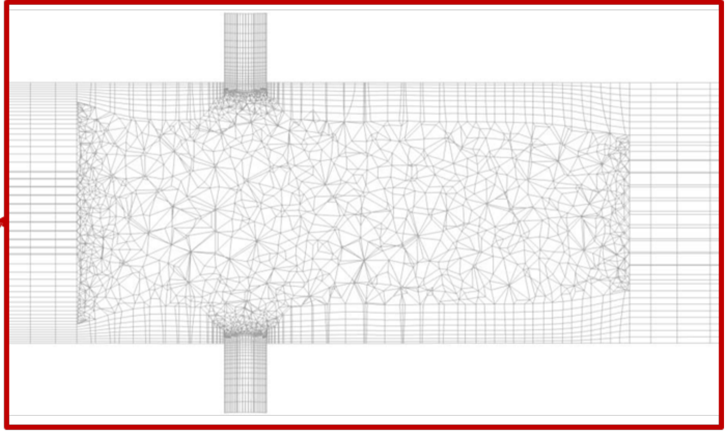
Validation by experimental results from Purdue

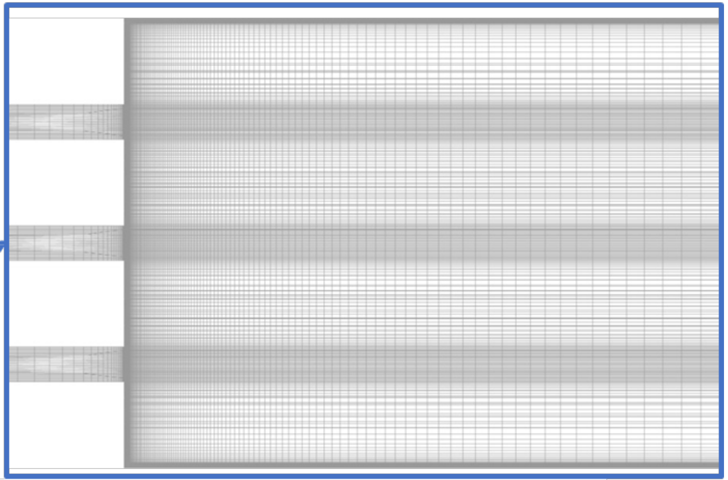
- Geometry: 19 fuel injection pipes and a combustion chamber
- Steady state RANS reacting flow simulation calculations

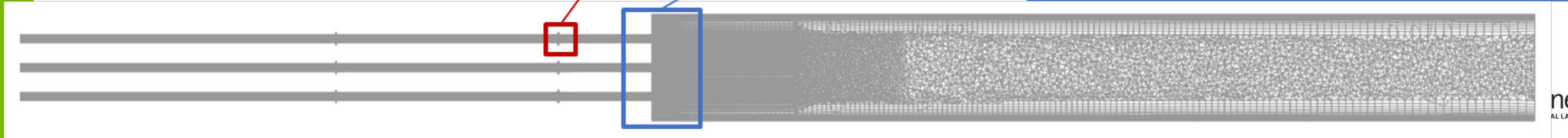
Chemical reaction mechanism: 25 species and 142 reactions

TASK 2: GRID OVERVIEW

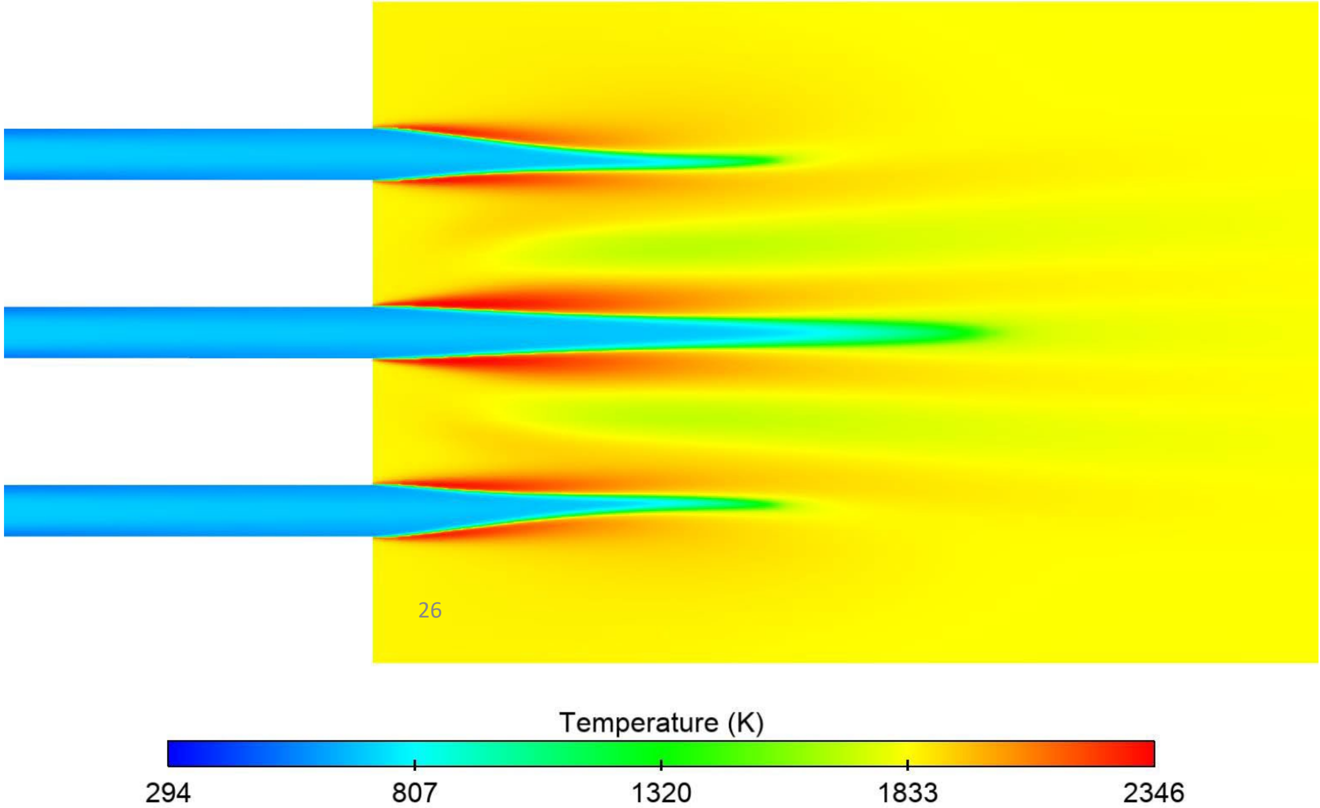
- Grid features:
  - ➢ Hybrid unstructured mesh
  - ➢ 11 million cells
  - ➢ Significant resolution required near injection holes
  - ➢ High resolution near posts required to resolve flame shape and obtain better numerical stability
  - ➢ Multiple grid iterations were required to accurately resolve flame and increase numerical stability



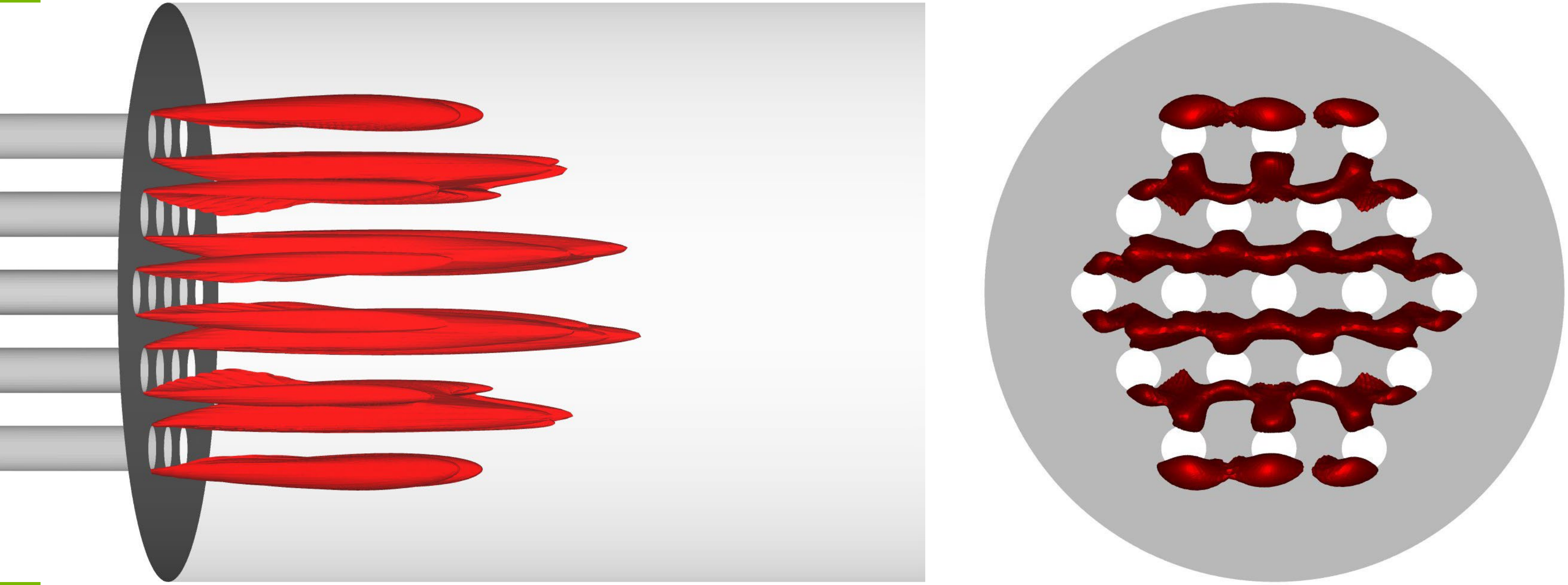




TEMPERATURE PLOT

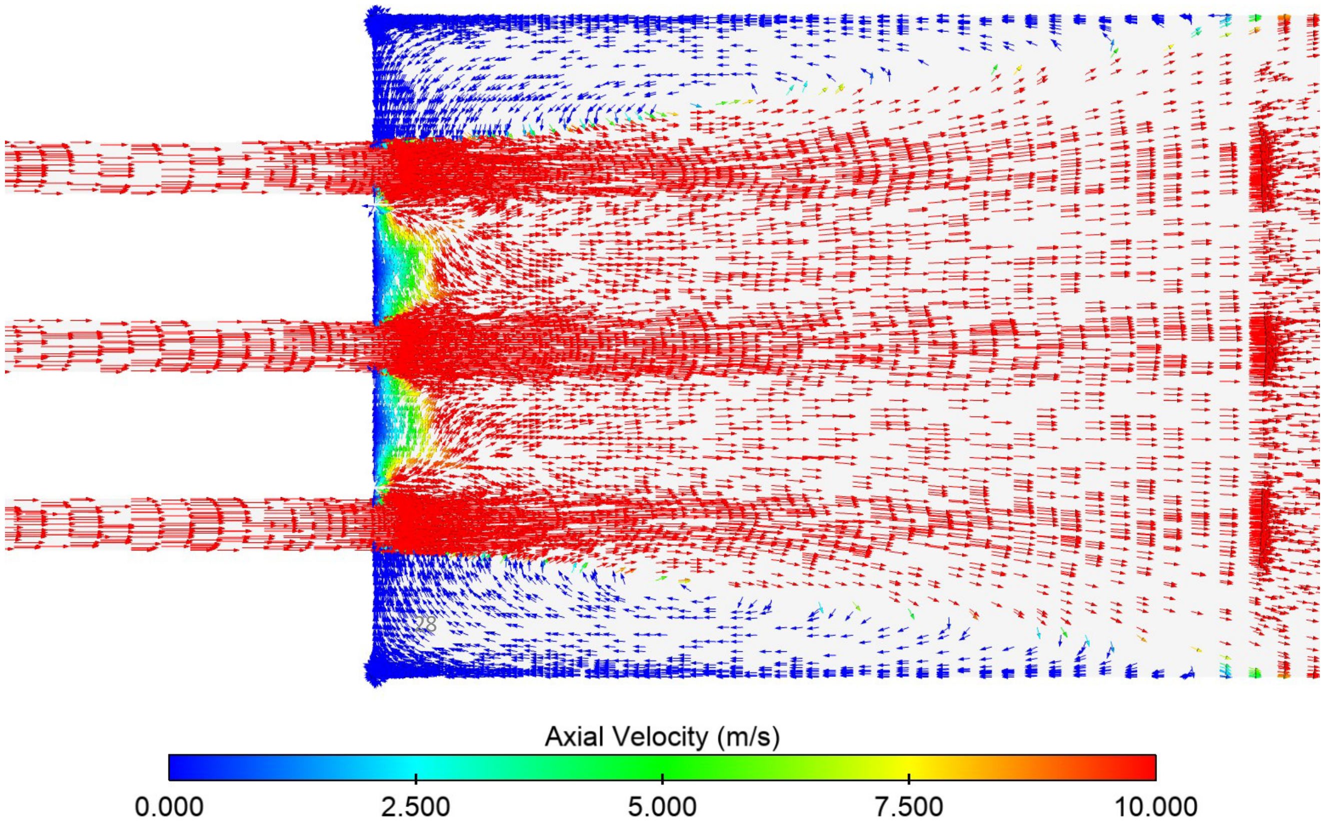


TEMPERATURE ISOVOLUME > 1900 K



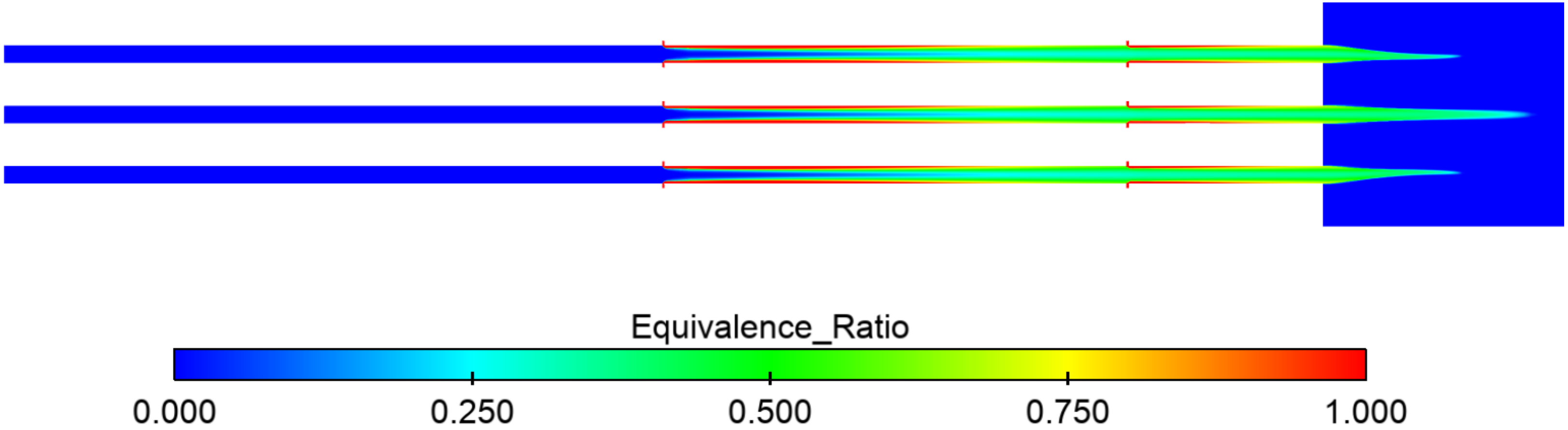
Unmixedness in H2 (shown later) causes high temperature only above/below injection pipes

VELOCITY VECTORS: RECIRCULATION ZONE VISUALIZATION



CRAFT Tech

EQUIVALENCE RATIO PLOT

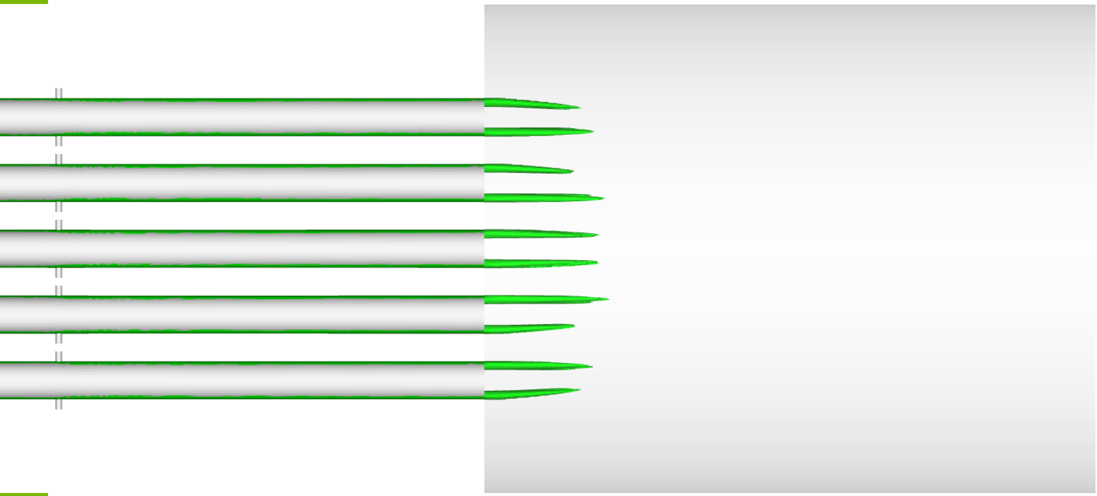


$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$$

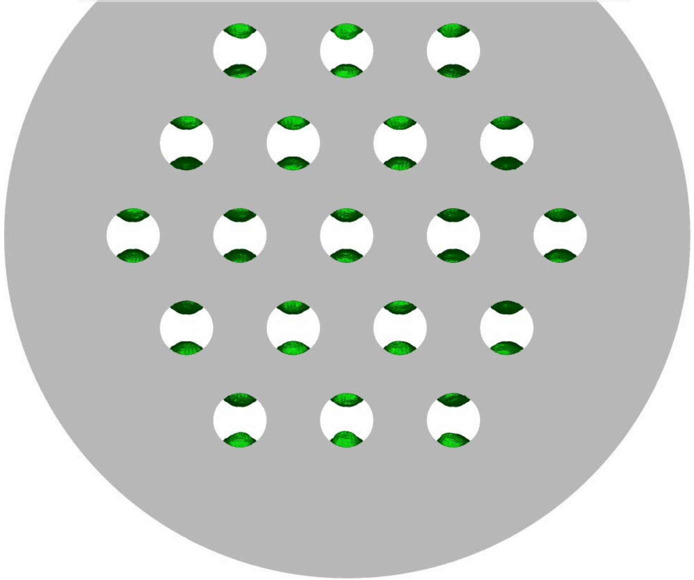
$$\left(\frac{F}{Ox}\right)_{stoic} = \frac{CH_4}{2O_2} = \frac{16.04}{64} = 0.25$$

$$\varphi = \frac{\frac{F}{Ox}}{\left(\frac{F}{Ox}\right)_{stoic}} = \frac{\frac{Y_{H2} + Y_{CH4}}{Y_{O2}}}{0.25}$$

EQUIVALENCE RATIO ISOVOLUME > 0.5



- View is from the back of the chamber (exit) looking in
- Gray surface is the face plate where pipes meet chamber



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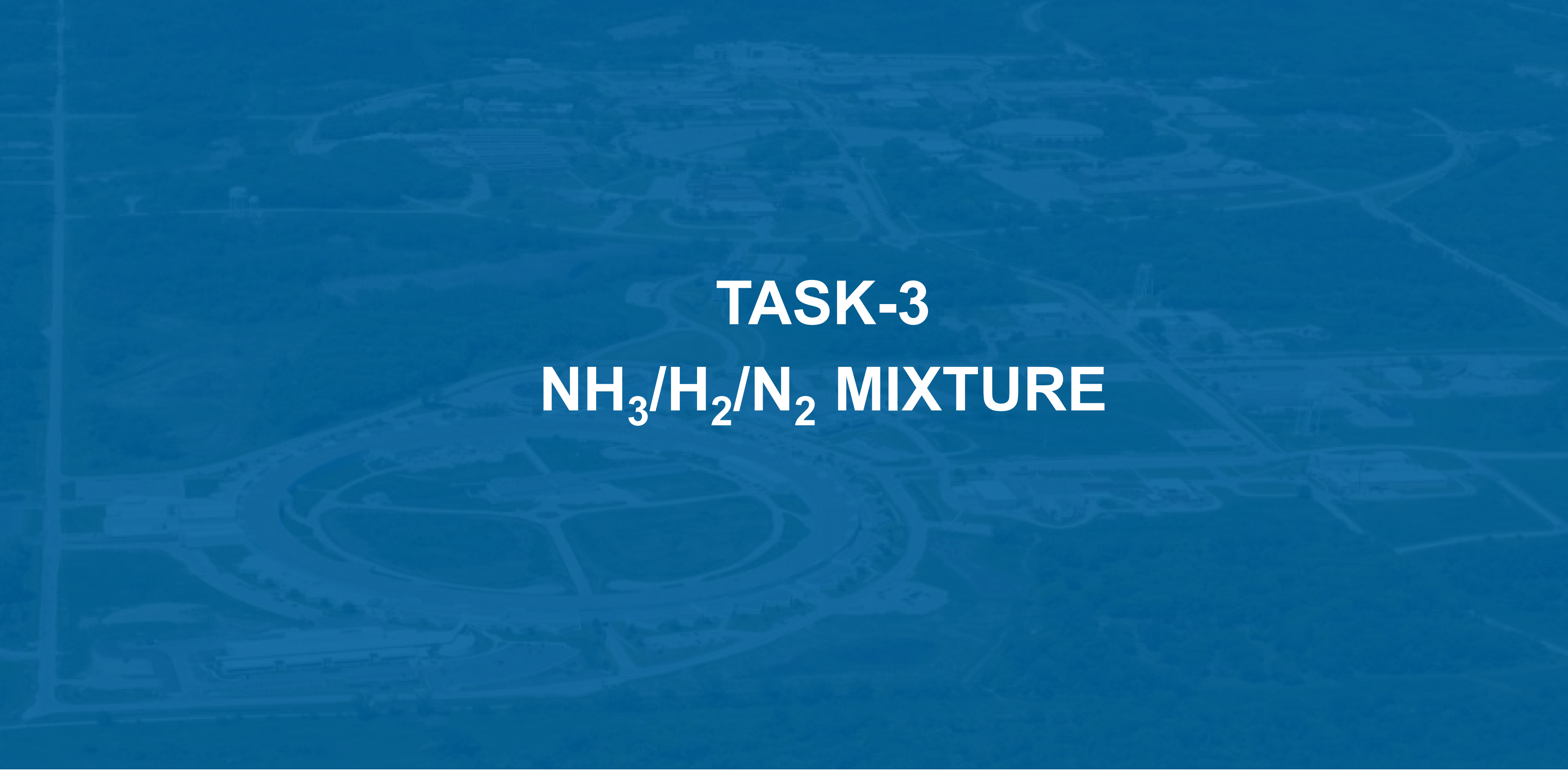


TASK-3

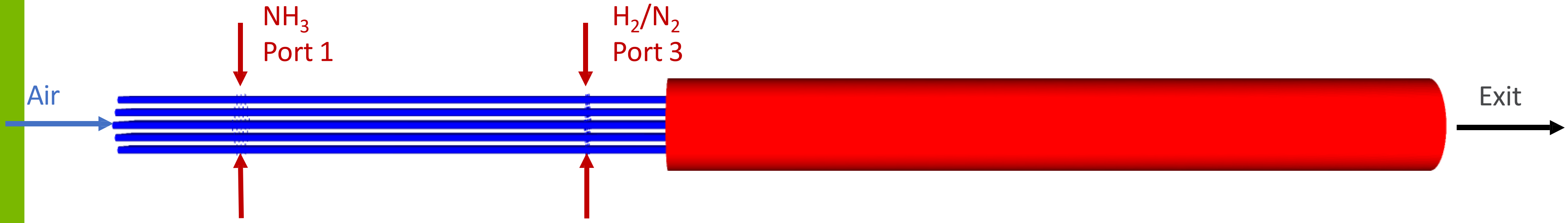
$NH_3/H_2/N_2$ MIXTURE

TASK 3 OVERVIEW: COMBUSTING SIMULATION ($NH_3/H_2/N_2$)

- Geometry: 19 fuel injection pipes and a combustion chamber
- Steady state RANS reacting flow simulation calculations
- Boundary Conditions:

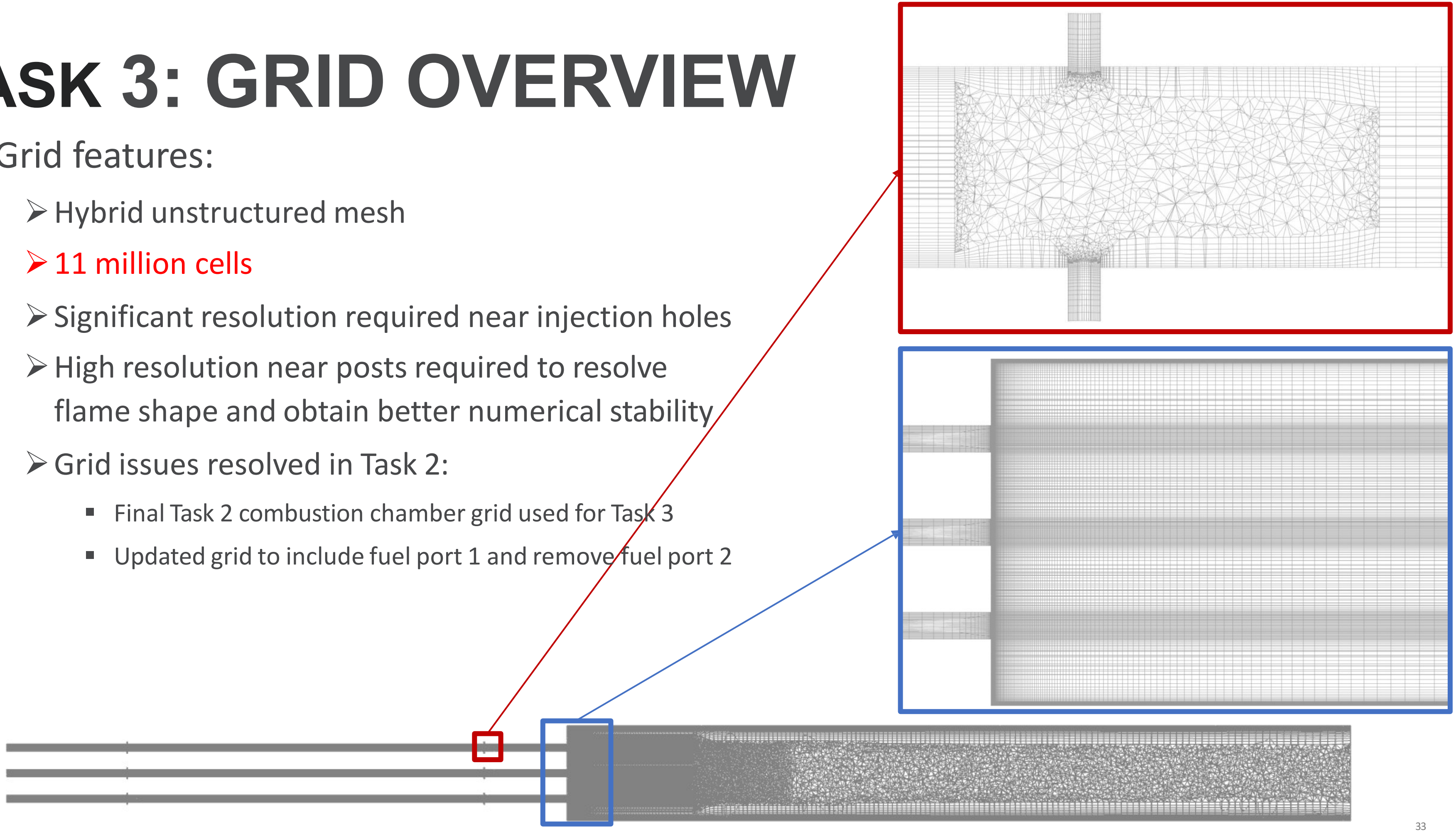
			Task 3		
			Case1 η = 0.4	Case2 η = 0.5	Case3 η = 0.6
	Fuel Composition		NH3/ H2/N2 mix	NH3/ H2/N2 mix	NH3/ H2/N2 mix
NH3 @ 305.4K	Fuel Inlet Mass Flow (Port 1)	kg/s	0.023638	0.01970	0.01576
H2 @ 294.3K	Fuel Inlet Mass Flow (Port 3)	kg/s	0.00280	0.00350	0.00420
N2 @ 294.3K	Fuel Inlet Mass Flow (Port 3)	kg/s	0.01296	0.01620	0.01944
	Oxidizer Inlet Mass Flow	kg/s	0.454	0.454	0.454
	Oxidizer Inlet Temp.	K	755.4	755.4	755.4
	Exit Back Pressure	MPa	0.573	0.573	0.573

Chemical reaction mechanism:
33 species and 251 reactions



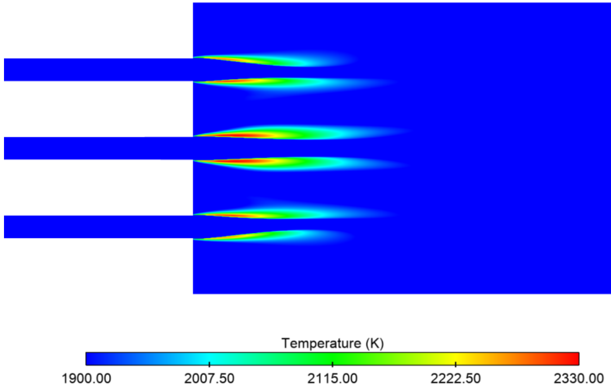
TASK 3: GRID OVERVIEW

- Grid features:
  - ➢ Hybrid unstructured mesh
  - ➢ 11 million cells
  - ➢ Significant resolution required near injection holes
  - ➢ High resolution near posts required to resolve flame shape and obtain better numerical stability
  - ➢ Grid issues resolved in Task 2:
    - ▪ Final Task 2 combustion chamber grid used for Task 3
    - ▪ Updated grid to include fuel port 1 and remove fuel port 2

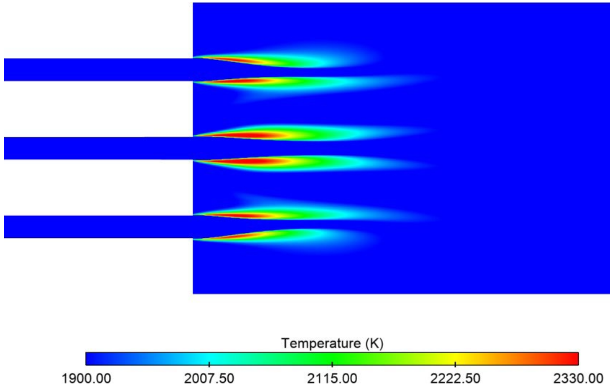


TEMPERATURE PLOT

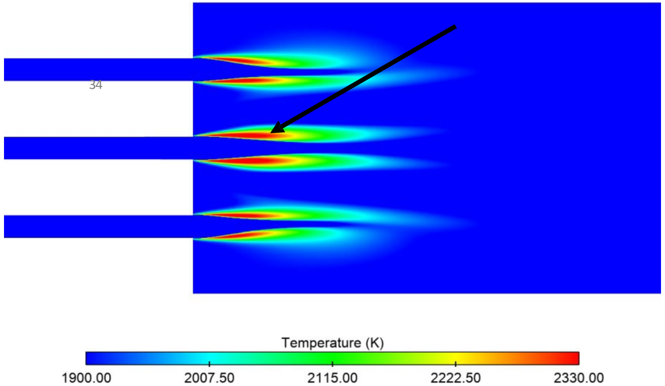
Case 1 (η =0.4)



Case 2 (η =0.5)



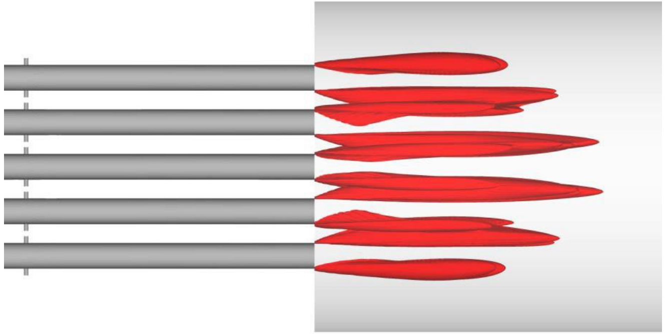
Case 3 (η =0.6)



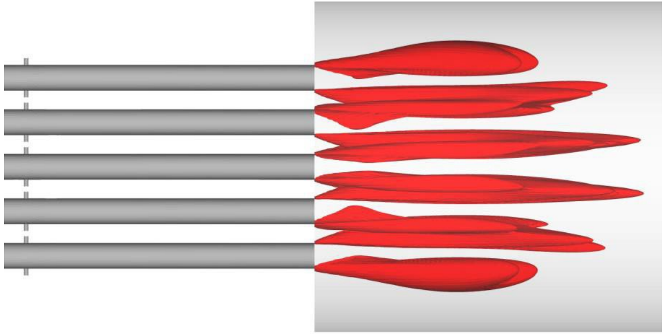
- Case 3 shows shortest flame
- Case 3 has larger higher temperature region surrounding flame

TEMPERATURE ISOVOLUME > 1900 K

Case 1 (η =0.4)

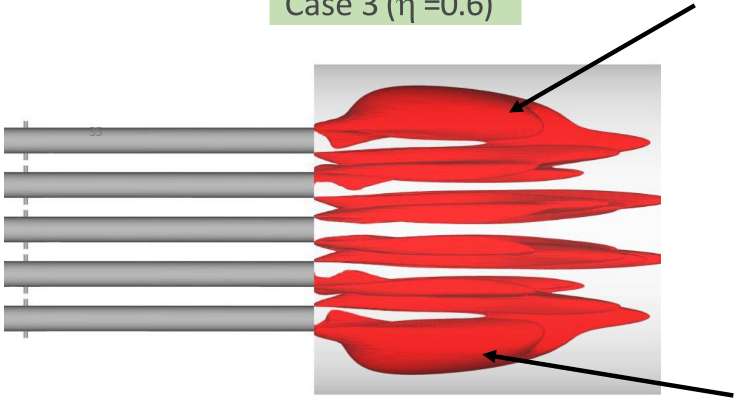


Case 2 (η =0.5)



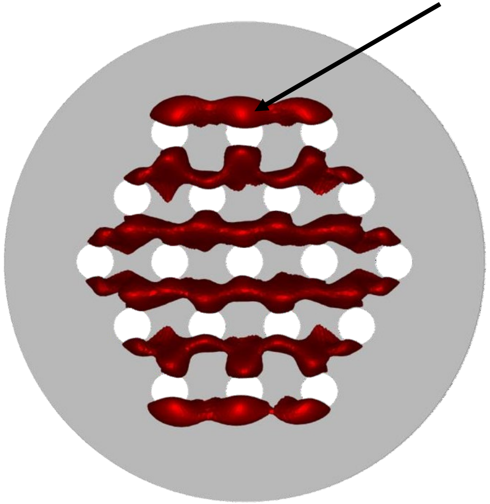
- Inner flames show similar temperature structure for all three cases except for length
- Top and bottom high temperature structure very different

Case 3 (η =0.6)

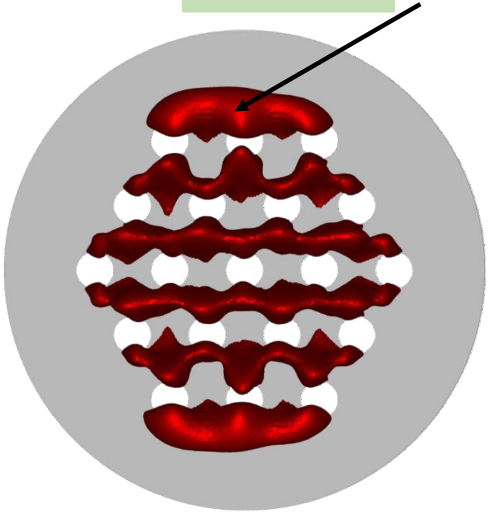


TEMPERATURE ISOVOLUME > 1900 K

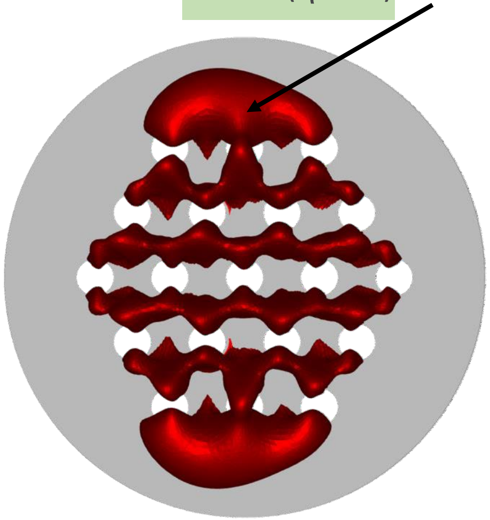
Case 1 (η =0.4)



Case 2 (η =0.5)



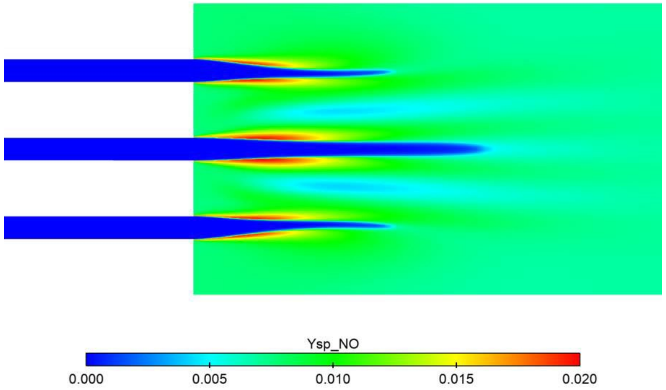
Case 3 (η =0.6)



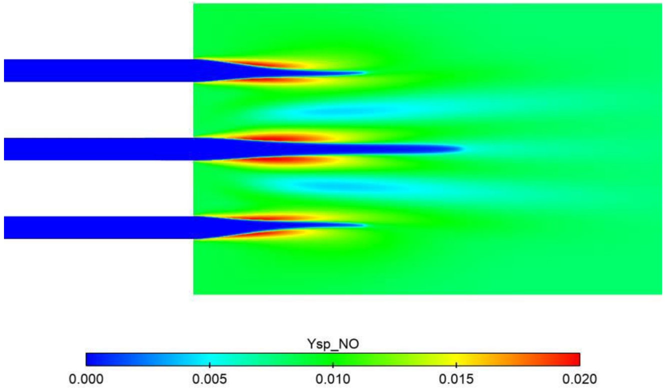
- View is from the back of the chamber (exit) looking in
- Gray surface is the face plate where pipes meet chamber
- Inner flames show similar temperature structure for all three cases except for length
- Top and bottom temperature structure very different

SPECIES PLOTS: NO MASS FRACTION

Case 1 (η =0.4)

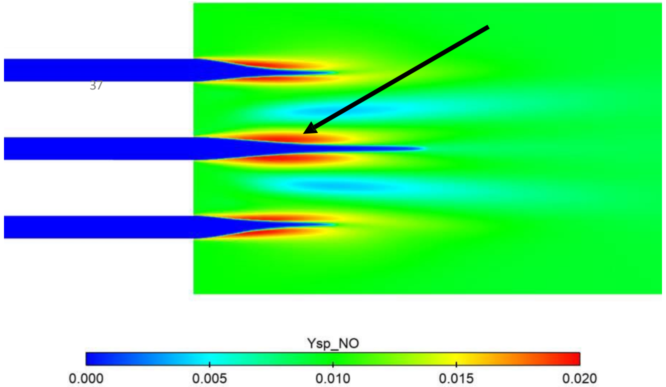


Case 2 (η =0.5)



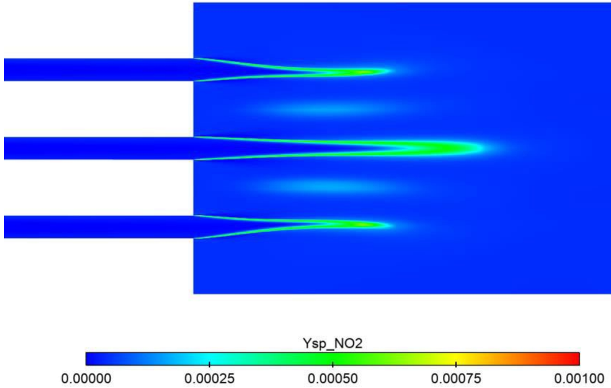
17,517 ppm

Case 3 (η =0.6)

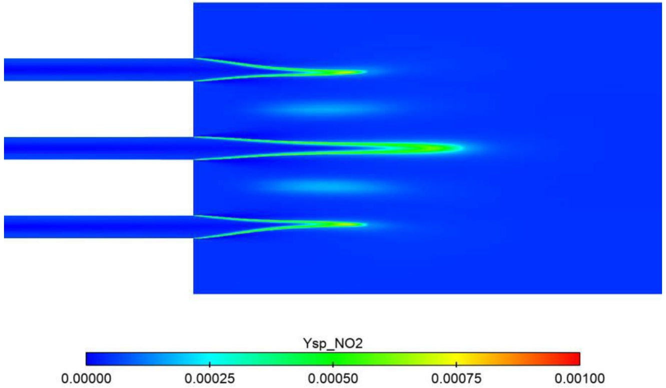


SPECIES PLOTS: NO_2 MASS FRACTION

Case 1 (η =0.4)

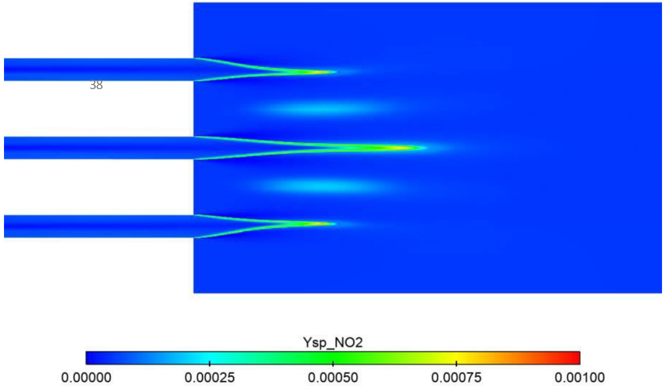


Case 2 (η =0.5)



571 ppm

Case 3 (η =0.6)



- NO2 shows outline of flame structure well
- Case 3 has shortest flame

COMPUTATIONAL COST

- All simulations were conducted on the Broadwell nodes on the mid-sized supercomputing cluster (Bebop) at ANL :
  - Strong scaling studies were performed to determine optimal number of nodes for each simulation.
  - Cold flow simulations were run on 108 cores (3 nodes) and took about 5 hours for convergence (achieving less than 0.1% mass error)
  - Reacting flow simulations were run on 360 cores (10 nodes).
  - Typical time for simulations were 8-10 days (200 – 240 hours) depending on the mechanism size.
  - Large amounts of computational resources are needed to accurately resolve the jet (high resolution mesh) and to obtain good mass flow convergence (< 0.1% error).

CURRENT STATUS

- **Design refinement using 1-D model (ongoing)**
- **CFD analysis to identify optimal fraction of dissociation (completed)**
  - Ideally, $0.4 < \eta < 0.7$

FUTURE TASKS

Phase-3: Fuel Preconditioner design & build (FY 24)

Phase-4: Demonstration in 1MW Combustor (FY 25)

THANK YOU!

Argonne
NATIONAL LABORATORY