Fundamental Experimental and Numerical Combustion Study of H_2 Containing Fuels for Gas Turbines

PI: Prof. Subith Vasu

Co-PIs: Prof. Artem Masunov[1], Dr. Scott Martin[2], Prof. Daniel Banuti[3], Prof. Robert P. Lucht[4]

[1]University of Central Florida, Orlando, FL

[2]Embry-Riddle University, Daytona Beach, FL

[3]University of New Mexico, Albuquerque, NM

[4]Purdue University, West Lafayette, IN

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PM: Matt Adams

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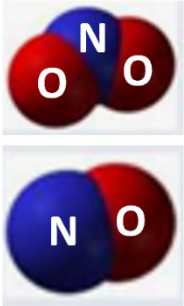
Contact: subith@ucf.edu

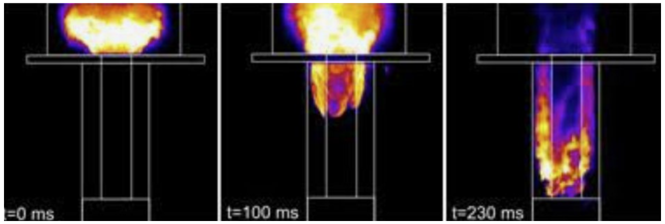
Introduction

- Some major challenges involved in hydrogen containing fuel combustion/ combustor development

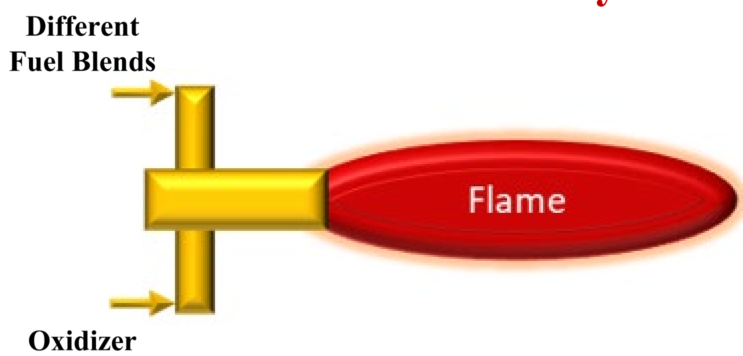
Thermal / Fuel NOx



Flashback



Fuel Flexibility



- Fundamental tools and knowledge must be advanced in order to improve or design new combustion chambers

Mixtures of Focus

- Various H_2 fuel combustors that are being developed by various OEMs

	Type	Notes	TIT ^{o}C [^{o}F] or Class	Max H_2 % (Vol)
MHPS	Diffusion	N2 Dilution, Water/Steam Injection	1200~1400 [2192~2552]	100
	Pre-Mix (DLN)	Dry	1600 [2912]	30
	Multi-Cluster	Dry/Underdevelopment - Target 2024	1650 [3002]	100
GE	SN	Single Nozzle (Standard)	B,E Class	90-100
	MNQC	Multi-Nozzle Quiet Combustor w/ N2 or Steam	E,F Class	90-100
	DLN 1	Dry	B,E Class	33
	DLN 2.6+	Dry	F,HA Class	15
	DLN 2.6e	Micromixer	HA Class	50
Siemens	DLE	Dry	E Class	30
	DLE	Dry	F Class	30
	DLE	Dry	H Class	30
	DLE	Dry	HL Class	30
PSM Ansaldo	Sequential	GT26	F Class	30
	Sequential	GT36	H Class	50
	ULE	Current Flamesheet™	F, G Class	40
	New ULE	Flamesheet™ -- Target 2023	Various	100

Current and near-term capabilities of OEMs for H2 containing fuel fired gas turbines (Ref: D. Noble et al., "Journal of Engineering for Gas Turbines and Power, 2020, doi: 10.1115/1.4049346)

Non-premixed combustor

N2 dilution, water/ steam injection
→ **Efficiency penalty with steam.**

Premixed type burners

- There are premixed, non-premixed, and also heavy N_2 diluted combustion strategies are in practice.
- Lean to Rich (H_2/NG/NH_3) mixtures in N_2 dilutions are primary interest

Team Co-ordination

DOE UTSR MANAGEMENT

SUBRECIPIENTS

Dr. Robert Lucht — PURDUE UNIVERSITY

(Counterflow flame Experiments: Strain Vs NOx)

Dr. Scott Martin — EMBRY-RIDDLE AERONAUTICAL UNIVERSITY

(Kinetics Reduction Based on Turbulence-Chemistry Interaction, CFD)

Dr. Daniel Banuti — THE UNIVERSITY OF NEW MEXICO

(DNS simulations for Turbulent Flame Speed and Mixing)

PRIME RECIPIENT

Dr. Subith Vasu (PI)

(Project Management, Autoignition, NOx & CO Measurements, Laminar Flame Speed, Detailed Chemical Kinetics, Oxidation and NOx Pathways, AI Tools)

Dr. Artem Masunov (co-PI)

(Chemical Kinetics, Reaction Rate Constants by Using Quantum Chemistry)

UCF UNIVERSITY OF CENTRAL FLORIDA

OEM/INDUSTRY ADVISORS

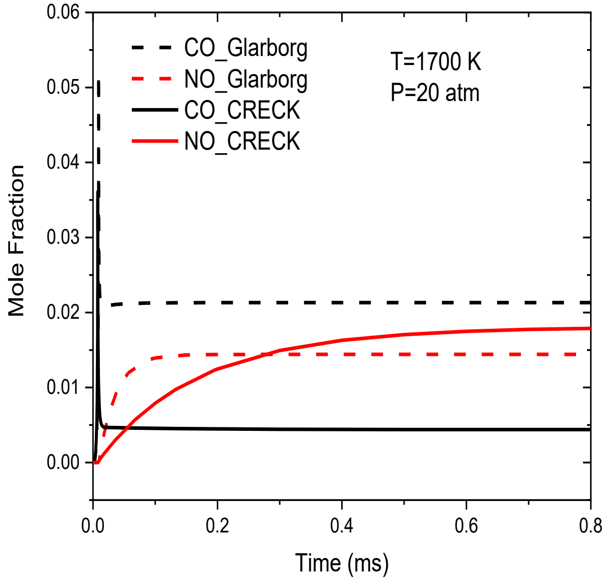
Dr. Carlos Koeneke — MITSUBISHI POWER

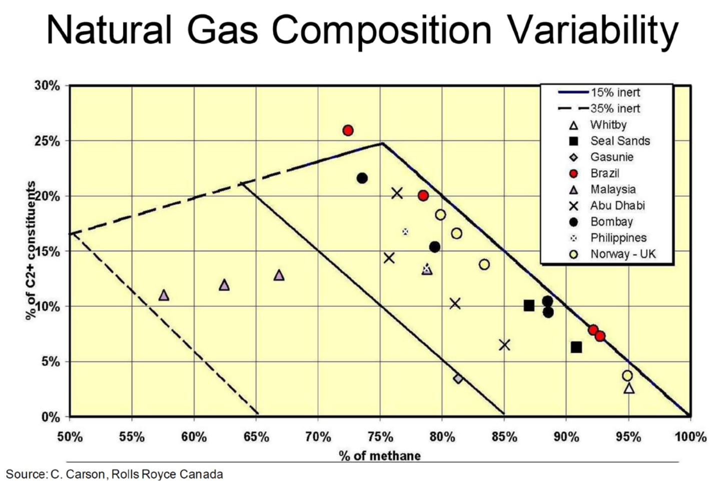
Dr. Keith McManus — GE

Fundamentals of Focus
(Chemical Kinetics)

Fundamentals of Focus- NOx formation during H_2/NG combustion

- Chemical Kinetics of H_2 containing fuels is being studied approximately from the past two decades. **However, discrepancy in the models still exists.**

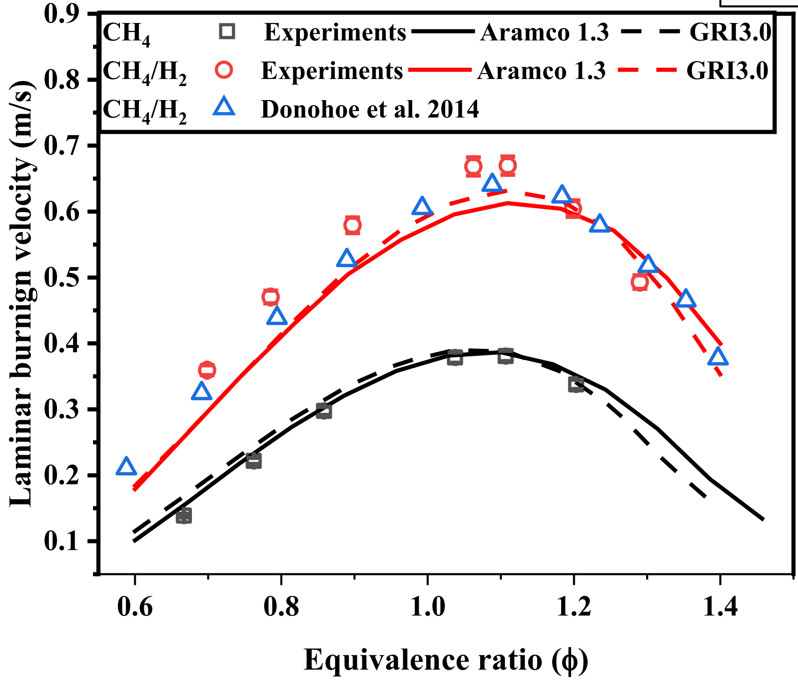


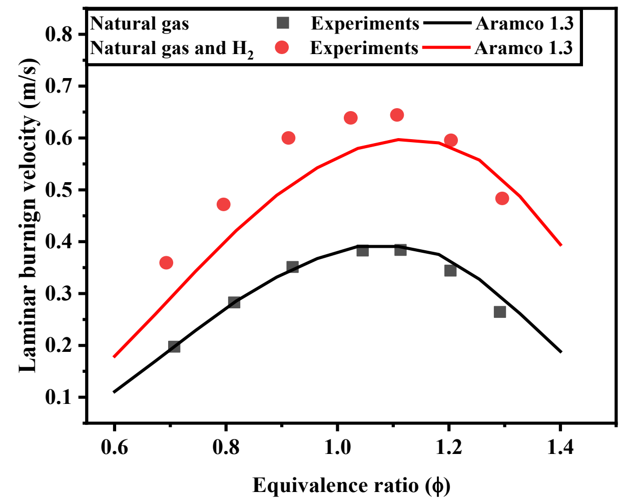


CO (black traces) and NO (red traces) formation time-histories from two recent NOx literature mechanisms, CRECK and Glarborg. **Considerable differences can be seen→need new experimental data for validation.** Mixture: 80% NG (90% CH_4/**10% C_2H_6), 20% H_2, phi=0.6 in air, 20% N_2 dilution.**

Fundamentals of focus–
Flame Speeds of H_2/CH_4/Natural gas

Data taken from Vasu Lab: Turbo Expo 2021



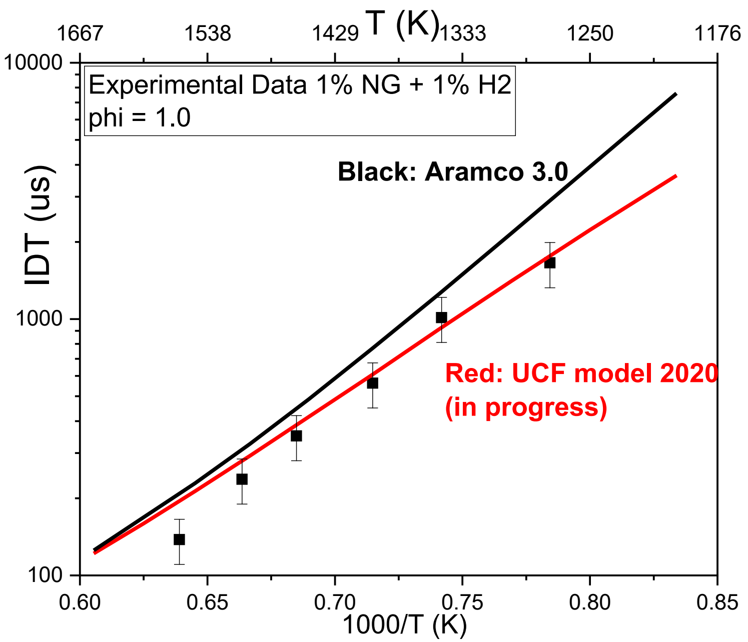


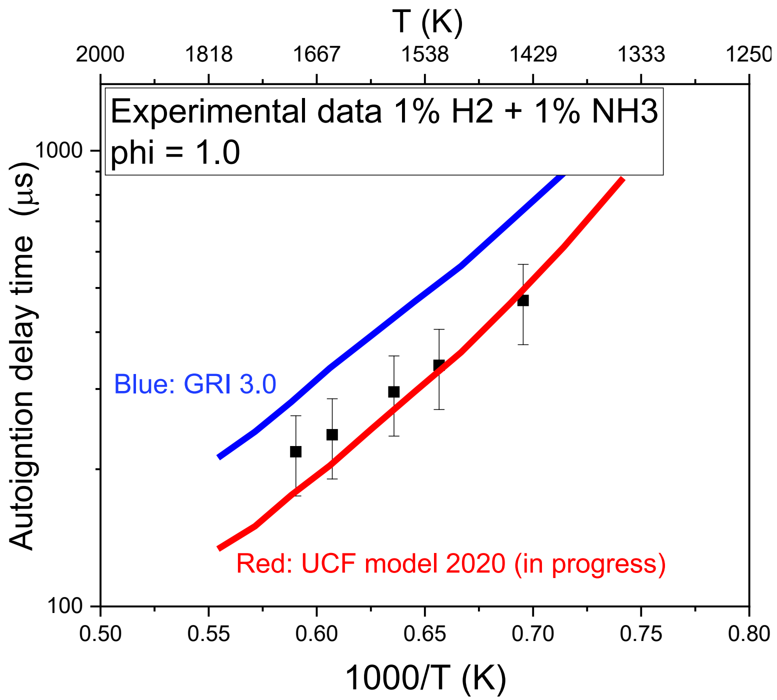
Discrepancies in predictions for natural gas/H2 mixtures

Pure methane/H2 mixtures are easily predicted by existing models

Need to look at this for specific compositions of interest to industry

Fundamentals of Focus



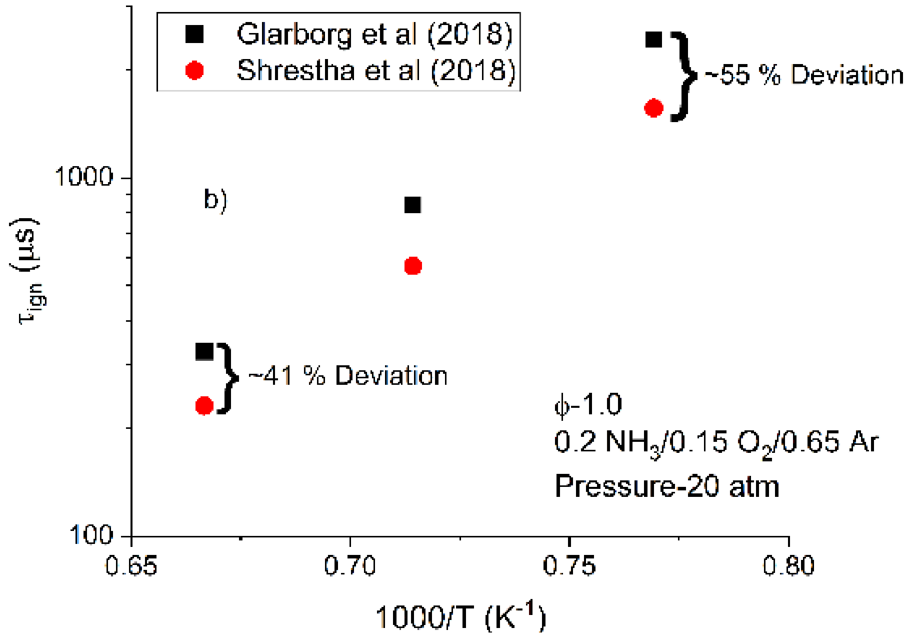


Experimental Ignition Delay Time data at ~ 2 atm, phi=1.0 (50% NG/ 50% H_2) and (50% NH_3/ 50% H_2) **(Experiments performed in Vasu's lab at UCF).** UCF model is work in progress.

- Chemical Kinetic models need improvement
- **Reasons for the limitations of existing kinetic models are in the next slide**

Fundamentals of Focus

Predictions of two recent ammonia chemical kinetic mechanisms (20% NH_3) near 20atm.



Clearly, this shows the uncertainty in predictions by the current state-of-the-art chemical kinetic models. This is because all these models were developed based on experimental results with lower concentrations of NH_3 (NH_3 as an impurity), and validation targets with experiments at higher concentrations are necessary when NH_3 is intended to be used as a fuel or fuel additive.

Fundamentals of Focus

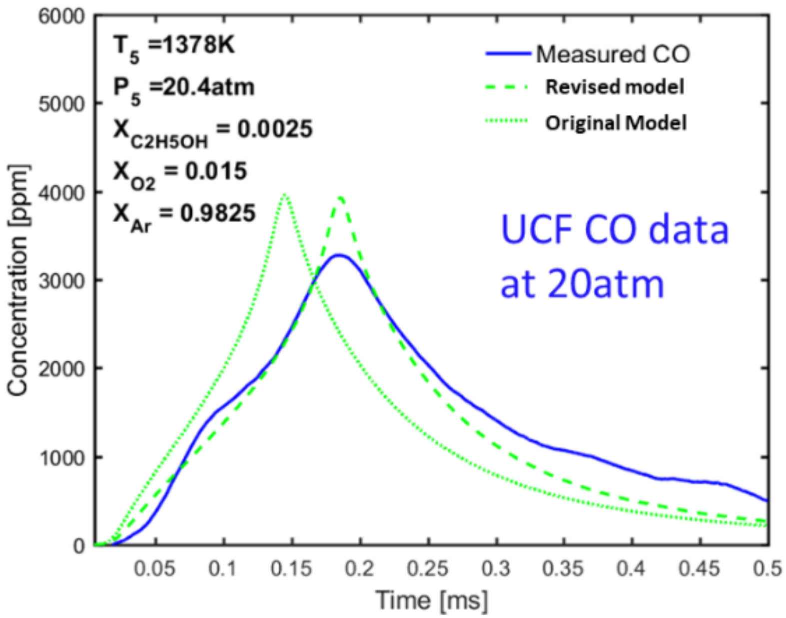
Chemical Kinetics:

- But here are the limitations of the existing hydrogen fuel kinetics:
  - ✓ Not validated against CO and NOx time histories
  - ✓ Not validated against rich mixtures
  - ✓ Not validated against high-fuel loadings
  - ✓ Not validated against high N_2 dilutions

- Thus, we are performing shocktube and laser speciation experiments to generate data to validate chemical kinetics
- Improve existing detailed kinetics if needed
- **Shocktube, Flame speed, and Chemical kinetic model improvements will be done at the UCF**

Fundamentals of Focus- Laser species measurements

CO time history measurements taken at the UCF near 20atm:



- UCF has significant experience in experimentally determining species time histories and modifying chemical kinetics

Fundamentals of Focus

Experimental Plan for Shock Tube Experiments:

Mixt.	Vol. % of H_2	Diluents	Measurements	Applicable to the OEM Combustors	Need for the study (additional details in the Merit Review Criterion Discussion)
H_2	90-100	N_2	NO	GE's MNQC; MHPS Multi-Cluster, Diffusion	Data not available in the literature
NH_3-H_2	10-90	No dilution	NO, IDTs	-	Current kinetic models not suitable at high-fuel loading; Models not validated with time resolved NOx data; H_2-NH_3 are not studied
H_2-NG	10-90	No dilution	CO, NO, IDTs	MHPS Pre-Mix; GE's DLN 1, 2.6+, 2.6e; Siemens DLE (E-HL class) Ansaldo Sequential, ULE	Current kinetic models are not suitable high-fuel loading conditions; Models not validated with time-resolved NO and CO data; Rich mixture for axial staging are not studied

Fundamentals of Focus

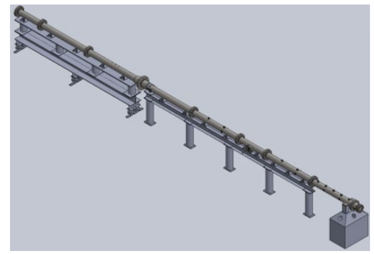
Experimental Plan for Flame Speed Experiments:

Mixt.	Targeted Measurements	Table 1 OEM Combustors	Need for the study (additional details in the Merit Review Criterion Discussion)
H_2-NG (10-90% Vol % H_2)	Laminar flame speed; Instability in expanding flame	MHPS Pre-Mix; GE's DLN 1, 2.6+, 2.6e; Siemens DLE Class E-HL; Ansaldo's Sequential, ULE	Flame speed data not available at high-fuel loading conditions; instability help to quantify influence of preferential diffusion
NH_3-H_2 (10-90% Vol % H_2)	Laminar flame speed; Instability in expanding flame		Flame speed data not available at high-fuel loading conditions; instability help to quantify influence of preferential diffusion

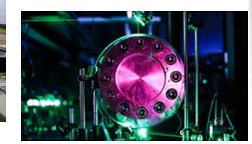
- **These flame speed experiments will be used for chemical kinetic model development and to develop other necessary correlations to use in combustor designs.**

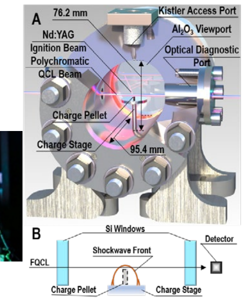
Vasu Lab Facilities for H_2/NH_3/Natural Gas Blends

2 Shock Tubes – realistic GT conditions with H_2/NH_3 permits



Laser and Optical Diagnostics

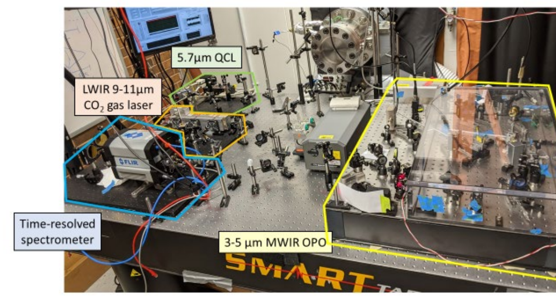




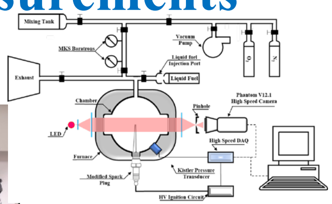
Capabilities

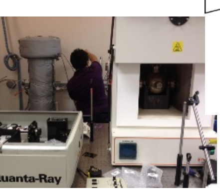
- High-Pressure Combustion up to 1000 bar and autoignition and emission species Measurements.
- Toxic impurities NOx, SOx, H_2S, and syngas
- Hydrogen or ammonia combustion with impurities
- Synthetic and biofuels
- Lasers for studying NOx formation routes
- High-Temperature Thermomechanical Response 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

UCF Shock Tube Laser Diagnostics



Flame Speed Measurements





Chemical Kinetic Modeling

Previous Collaborative Accomplishments

- **Aramco 3.0-** most comprehensive natural gas mechanism
- **UCF model for oxy-combustion SCO2-** most accurate model used by industry (GE, SWRI, Hanwha, KEPCO, CRAFT Tech) and DOE (NETL, NREL)
- **JetSurF model-** For jet fuel combustion used by OEMs

Absorption Measurements:
Beer-Lambert Law

$$\alpha = -\ln\left(\frac{I}{I_0}\right) = \sum_i \sum_j S_{ij}(T) X_j P L \phi_{ij}\left(\nu - \nu_{0_{ij}}\right)$$

I = Transmitted Intensity $\left(\frac{W}{cm^2 sr Hz}\right)$

I_0 = Incident Intensity $\left(\frac{W}{cm^2 sr Hz}\right)$

S_{ij} = Linestrength $\left(\frac{cm^{-2}}{atm}\right)$

T = Static Temperature (K)

X_j = Mole Fraction

P = Static Pressure (atm)

L = Path Length (cm)

ϕ_{ij} = Lineshape Function (cm)

ν = Optical Frequency (Hz)

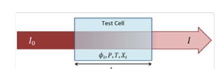
$\nu_{0_{ij}}$ = Line Center Optical Frequency (Hz)

Subscripts

i = Quantum Transition

j = Atomic/Molecular Species

(red)	Raw Sensor Data
(blue)	HITRAN/HITEMP/PNNL Databases, UCF Lab
(green)	PCB/CTAP –or- TDLAS
(black)	Hardware Constraint/Constant
(yellow)	Processed Sensor Data
(purple)	TDLAS velocity measurements

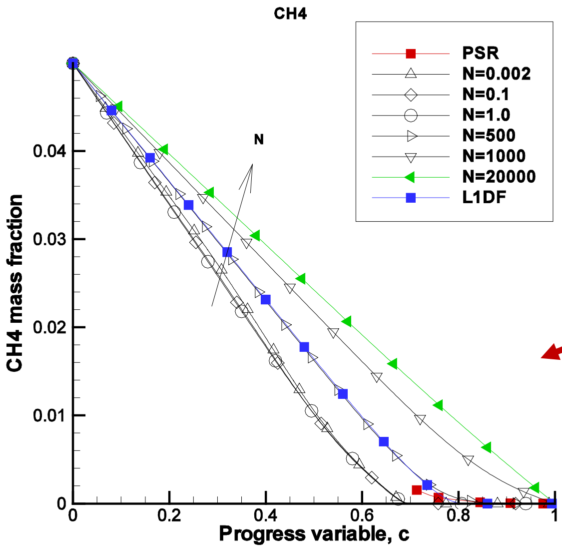


Fundamentals of Focus
(Reduced Chemical Kinetics)

Fundamentals of Focus

Reduced Chemical Kinetic Models for CFD :

- Reduced mechanisms for industrial use:
  - ✓ Existing chemical kinetic reduction models do not account turbulence-chemistry interactions
  - ✓ We use inhouse Premixed Conditional Moment Closure Model (PCMC) from ERAU to investigate turbulence and chemistry interactions and develop reduced kinetic models based on that



Variation in CH_4 oxidation with respect to scalar dissipation (N s^{-1}).
(N represents the local turbulence.)

Effect of Turbulence on Chemical Kinetic Pathways

Fundamentals of Focus
(Counter Flow Flame Studies)

Fundamentals of Focus

Relation between NOx and Flame strain

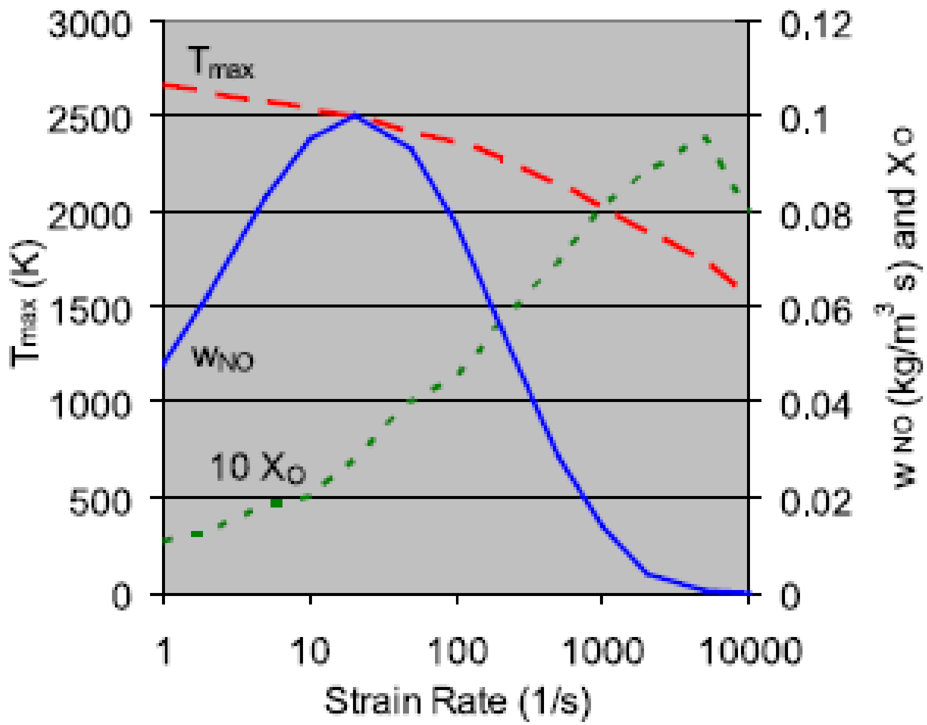


Figure adopted from **NETL online** publication Gas Turbine Handbook: Combustion Strategies for Syngas and High-Hydrogen Combustion; and J. P. H. Sanders, J. Y. Chen, and I. Gökalp, "Flamelet-based modeling of NO formation in turbulent hydrogen jet diffusion flames

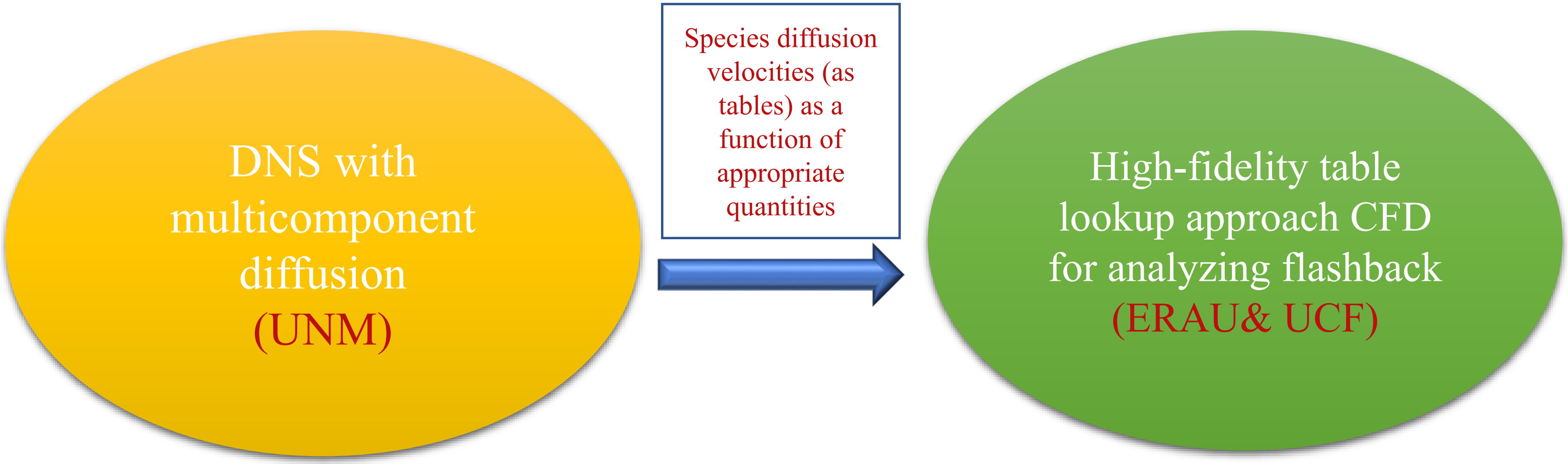
- Strain beyond certain extent can reduce the NOx formation.
- We perform these studies experimentally
- Purdue (Prof. Lucht) is performing this task

Fundamentals of Focus (Rapid Tools for Estimating H_2 Containing fuel Combustion Characteristics, e.g., Tools for Flashback Prediction)

Fundamentals of Focus

H_2 can diffuse much faster than heat (Le≠1)

- H_2 diffusion play can play a role in boundary layer flash back
- Including detailed multicomponent in combustion codes to predict flash back



Fundamentals of Focus (Rapid Tools for Estimating H_2 Containing fuel Combustion Characteristics)

Fundamentals of Focus

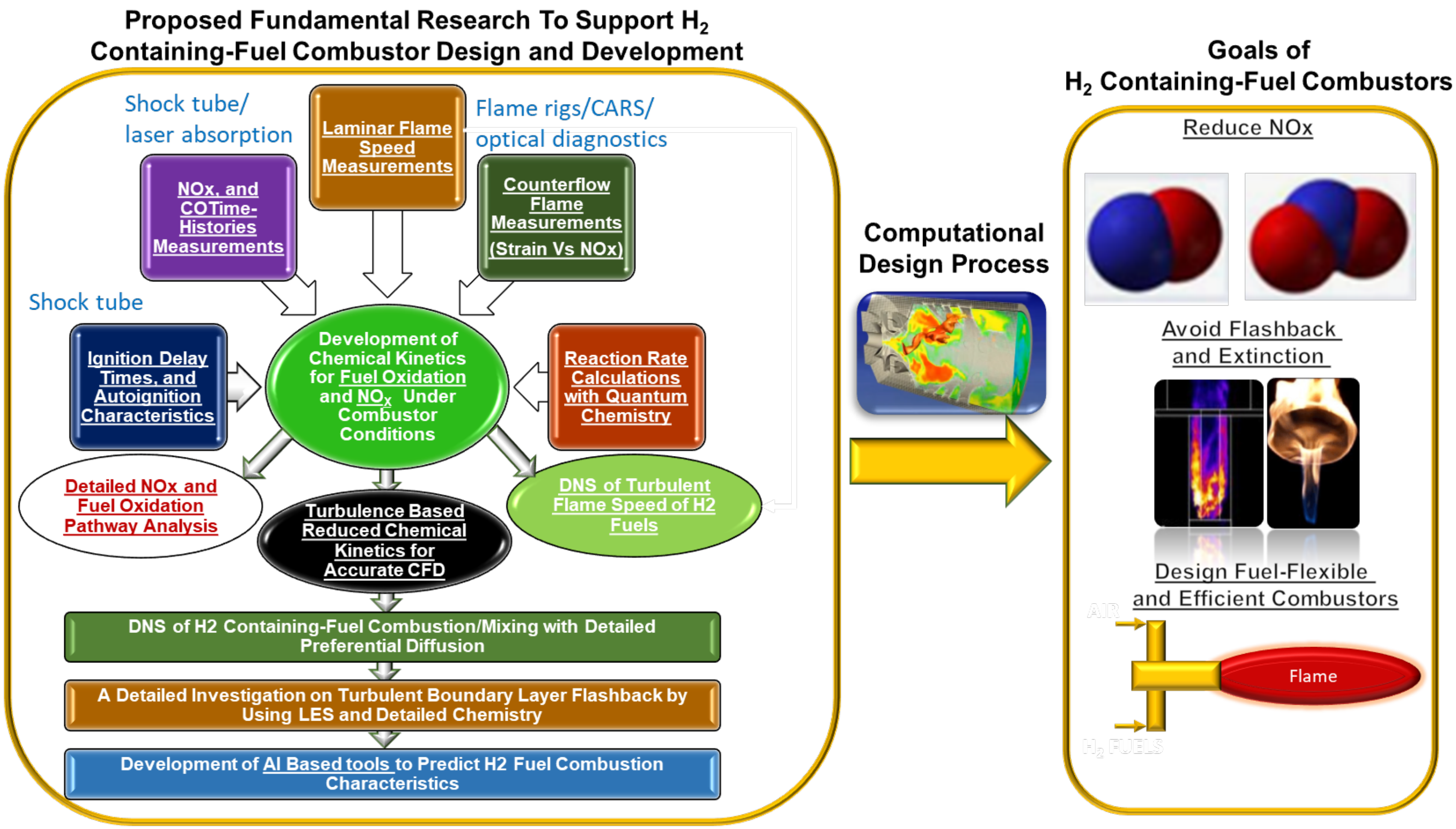
Deep Learning tools to help combustor design and troubleshoot

- Knowledge of **<u>all</u>** **<u>fundamental characteristics</u>** of a fuel blend is vital to accurately design or troubleshoot a combustor
- Unfortunately, it takes a huge time to estimate all the characteristics
- We train DL tools so that they can provide the necessary information to the user quickly
- We will obtain all the necessary training data from various high-fidelity 0-D, 1-D, CFD, and experimental models
- Special partnership with Microsoft

Microsoft

A Summary of the Project

Summary of effort



This project aims to fill the existing knowledge gaps and investigate the fundamental aspects of H_2 containing-fuel combustion to enable improved computational modeling for current and future gas turbine combustors developed and targeted by the leading original equipment manufacturers (OEMs).

Questions? Thank you