# Gaseous Fuel Interchangeability Criteria Development

## (CEC Contract 500-08-034; Marla Mueller)

**Vince McDonell, UC Irvine**

**California Energy and Air Quality Virtual Conference Series –**
***Air Quality Implications of Increasing Alternative Fuel Use***

**2 Nov 2010 Webinar**
**University of California, Irvine**

# Project Overview

- **"Interchange" is generally terminology associated with supply side….**
  - **"Wobbe Index": how many BTUs through a given hole at a given pressure—no combustion context**
- **Current project—focusing on utilization side**
  - **Design guides for how combustion systems perform/behave when fuel type/composition varies**
    - **Stand alone or sub-models for CFD simulation**
    - **Increasing penetration of intermittent renewable energy**
  - **Challenges for equipment/how to address?**
  - **What are the implications for environment?**
  - **Broader view vs LNG/natural gas**

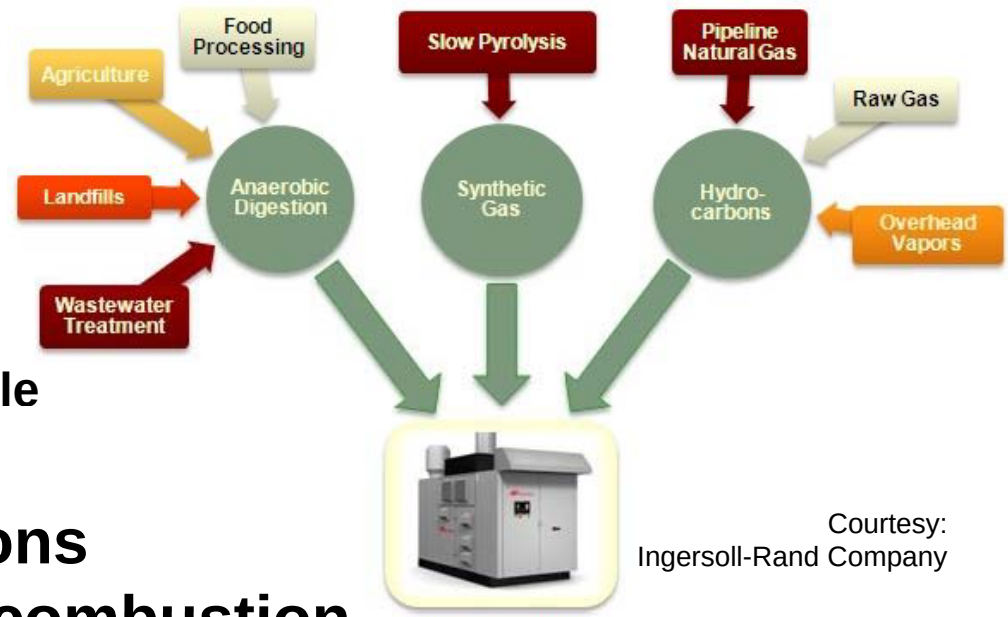
….”As we enter this new era of supply diversity, we must challenge the research of the past as we apply today's science and experience toward clarification of the possible uncertainty of the interchangeability results for current evaluations…” (Halchuk-Harrington and Wilson, 2006—commenting on AGA Bulletin #36)

# Project Overview

- **Example guides: correlations / relations / methodologies for**
  - **Ignition Delay time [fuel type, composition, conditions]**
    - **Keys--reaction rates, induction time, ……**
  - **Flashback Propensity [fuel type, composition, conditions]**
    - **Keys--Turbulent flame speed, diffusivity, quenching, strain….**
  - **Stability Limits [fuel type, composition, conditions]**
    - **Keys--Time scales, turbulent flame speed, reaction rates, strain….**
  - **Criteria pollutant emissions [fuel type, composition, conditions]**
    - **Keys--Kinetics, mechanisms, reaction rates, time scales….**
- **Stand alone guides or "hybridized" with CFD / simulation platforms**
  - **Models to assess/infer how equipment responds**

# Motivation

- **Use of gaseous fuels other than natural gas needs evaluation relative to potential societal benefits:**
  - **GHG**
  - **Air Quality**
  - **Cost of Electricity**
  - **Energy assurance**
    - **Diversity**
    - **Potential as a renewable**

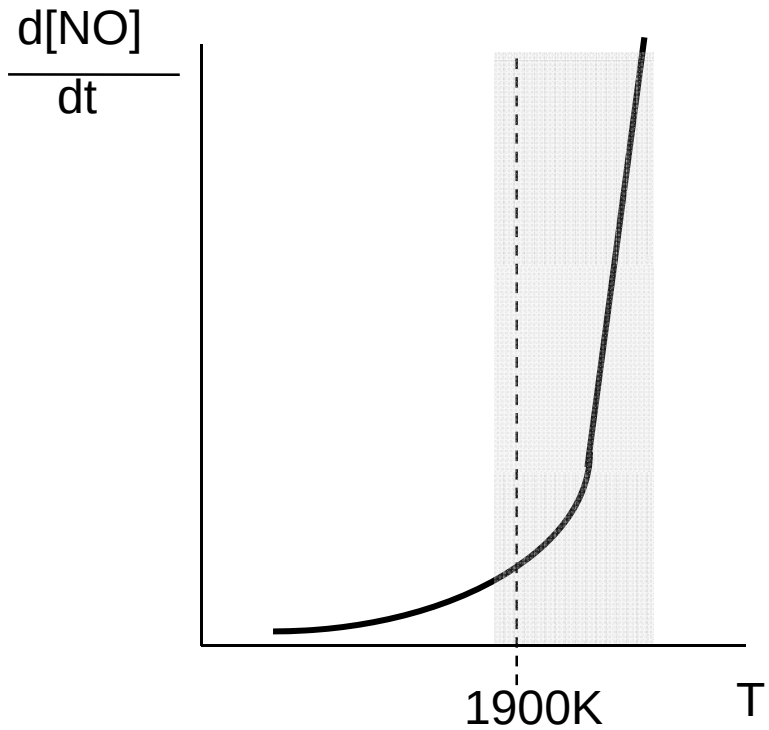


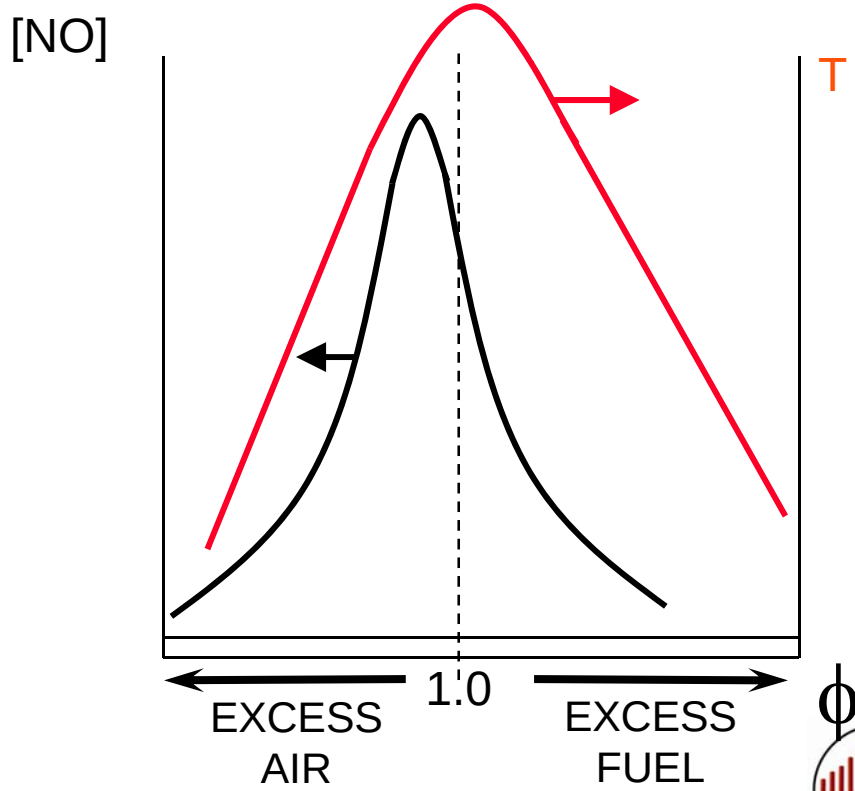

Courtesy:
Ingersoll-Rand Company

- **What are the implications of using such fuels in combustion systems?**
  - **Strategies for efficiently designing low emission systems requires understanding of key physical processes**

# Background

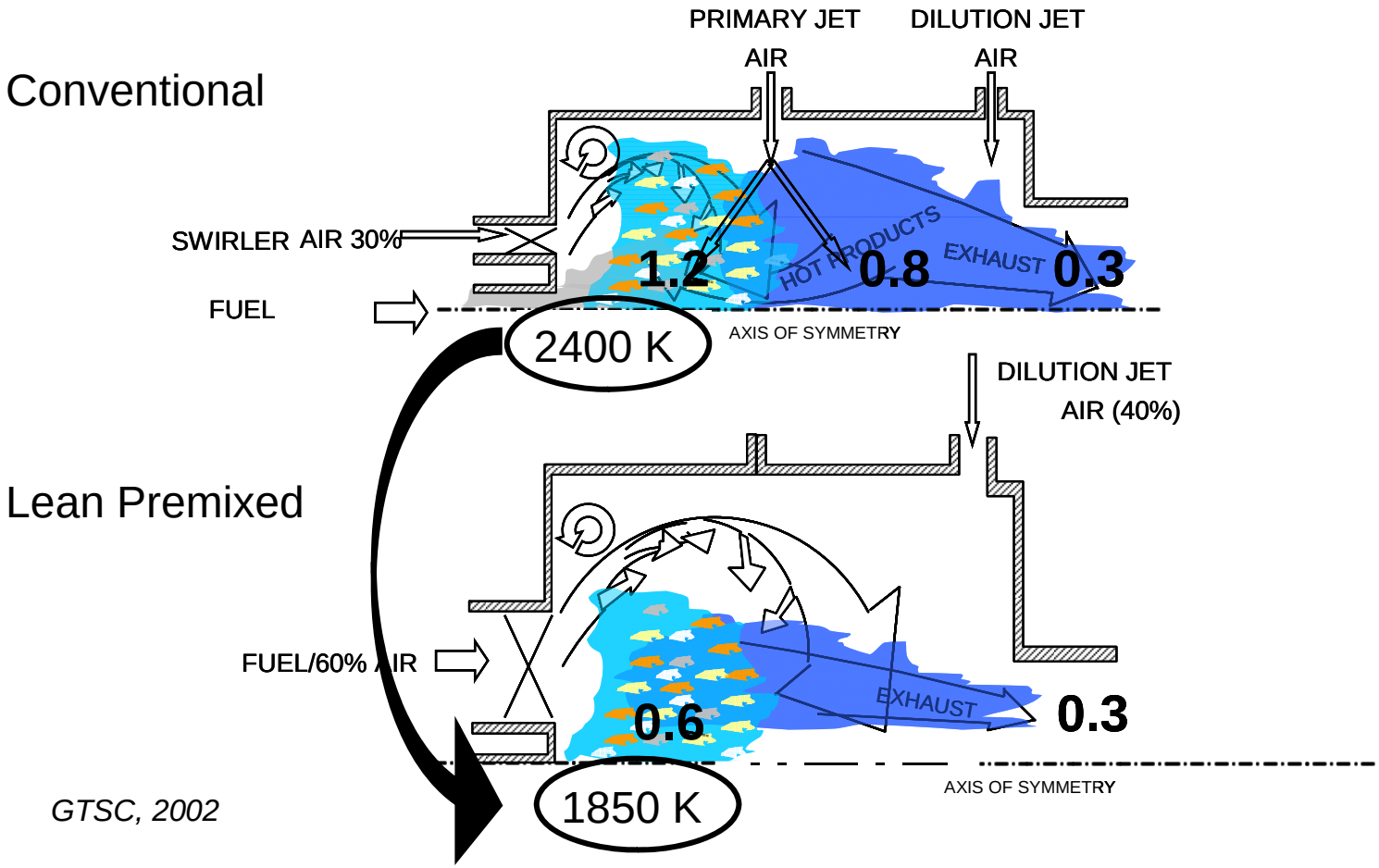
- **The pathway to low emissions….**
  - **All advanced combustion systems have achieved low NOx by avoiding combustion temperatures above 1900 K**
  - **Majority have focused on excess air strategies (i.e., fuel lean)**



# Background

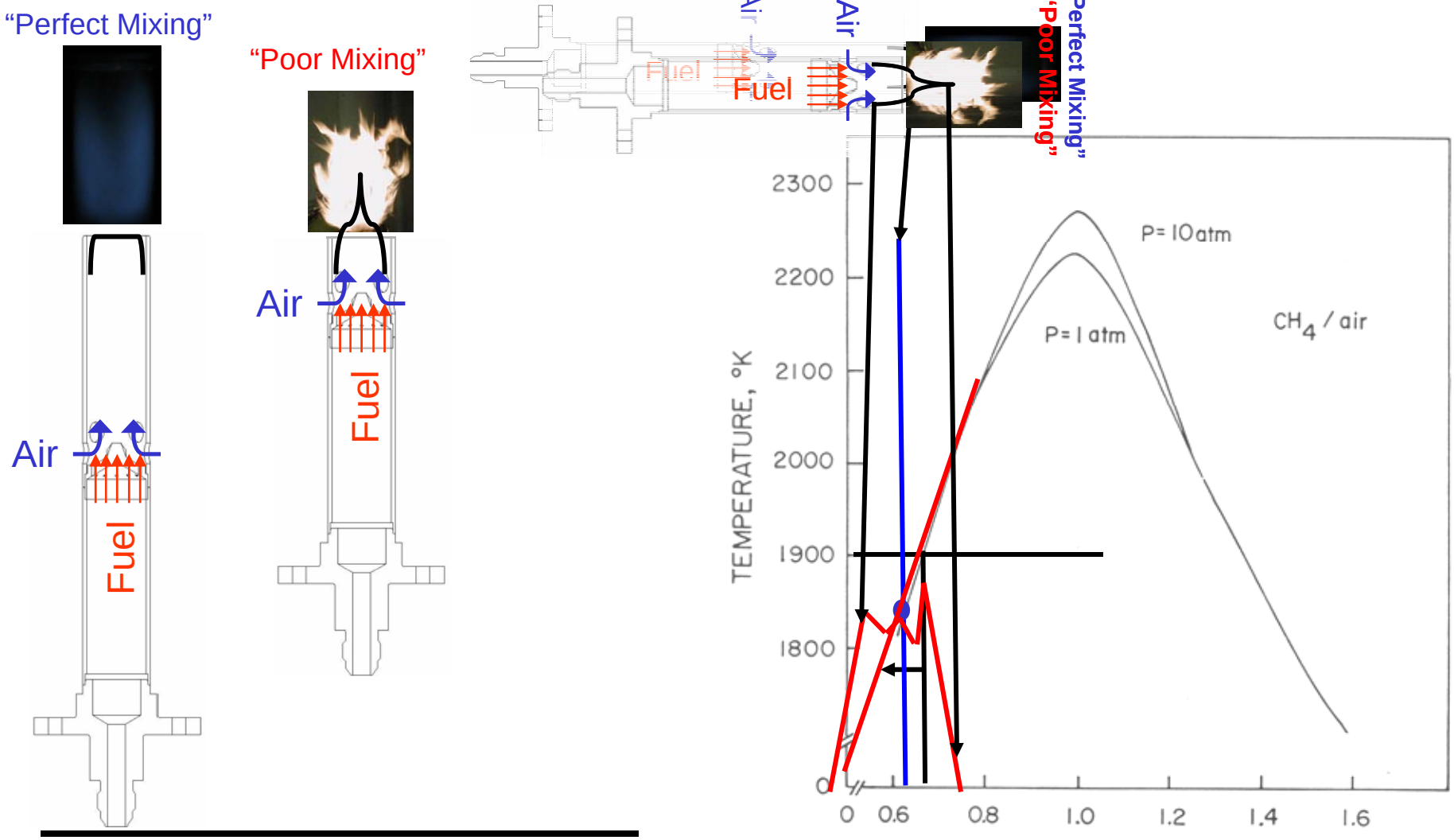
- **Lean Operation→potential to reduce T, NOx**




*GTSC, 2002*

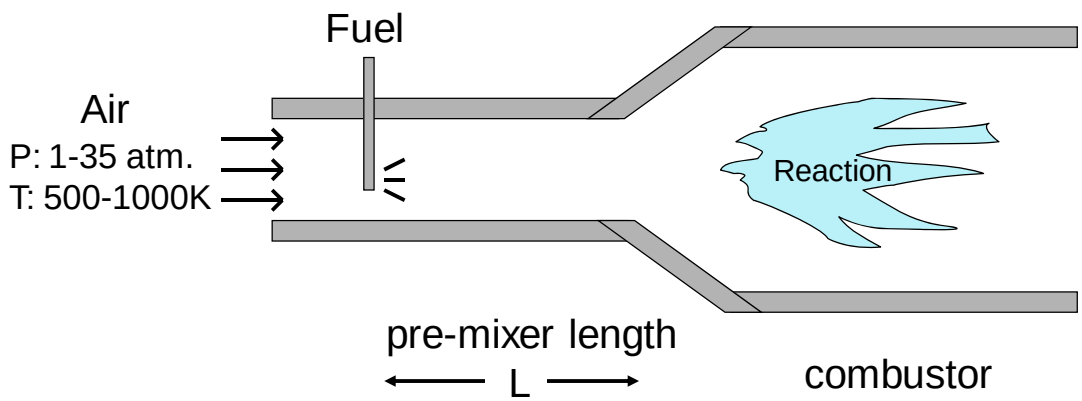
# Background

- **Mixing Key**



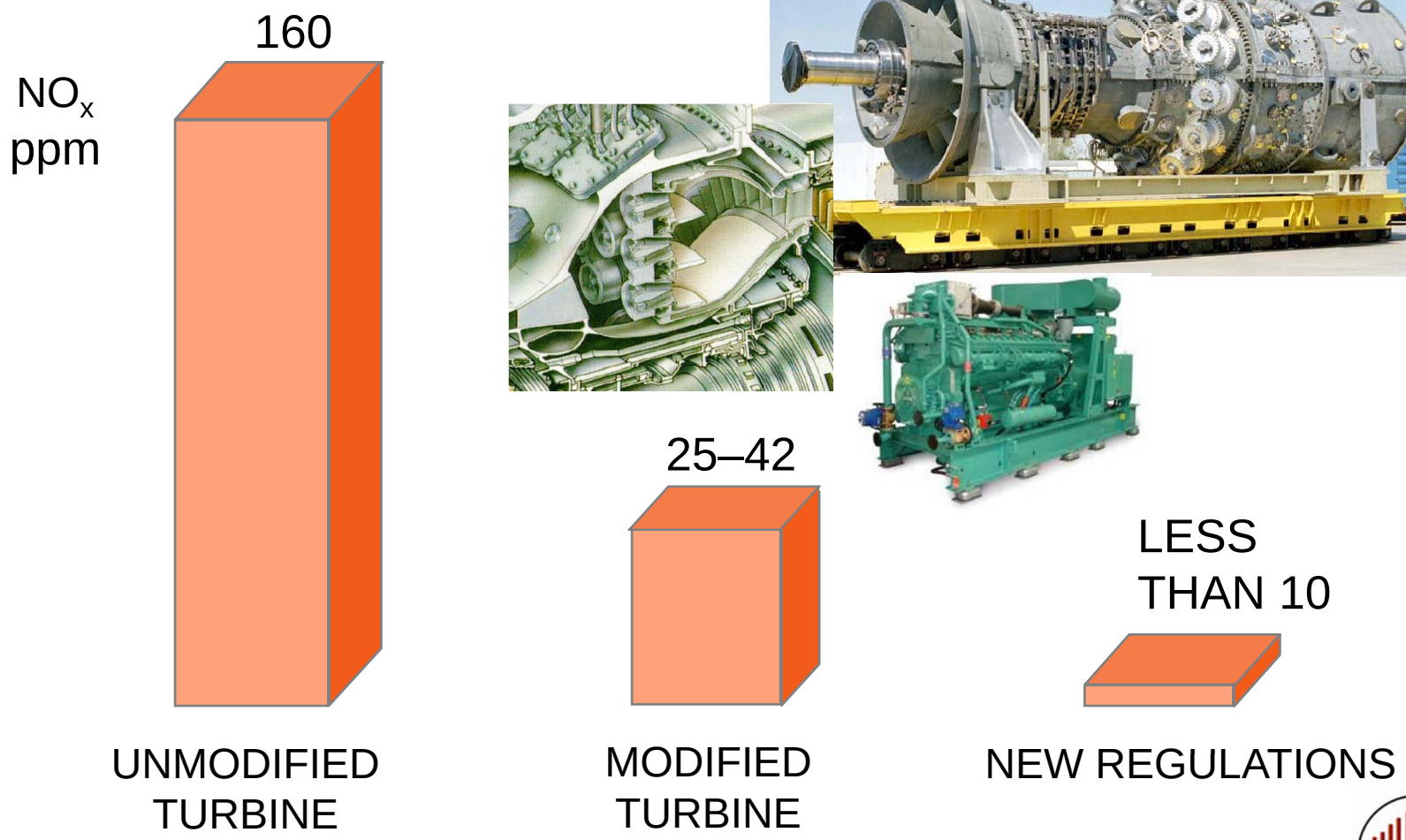
# Background

- **For success, a lean premixed system must:**
  - **Achieve uniform mixing to avoid "hot spots" in the reaction**
    - **NOx formation is exponentially dependent on temperature**
      - A small "fuel rich packet" can lead to considerable jump in NOx formation/emissions
- **Logical strategy: maximize time available for mixing of fuel/air prior to combustion**
  - **High temperature, high pressure environment→autoignition?**
  - **Keep reaction out of mixer→flashback?**



# Background

- **Progress over 30 years…..**



# Background

- **Success thus far has benefited by use of "single fuel" and optimization for single condition (e.g., full load)**

- **New paradigms**
  - **Fuels other than natural gas**
  - **Anticipation of higher transient operation**
    - **Load following for DG generation**
    - **Grid balance for large scale generation**

- **Key questions:**
  - **How does changing fuels impact operability?**
  - **How does changing fuels impact emissions?**

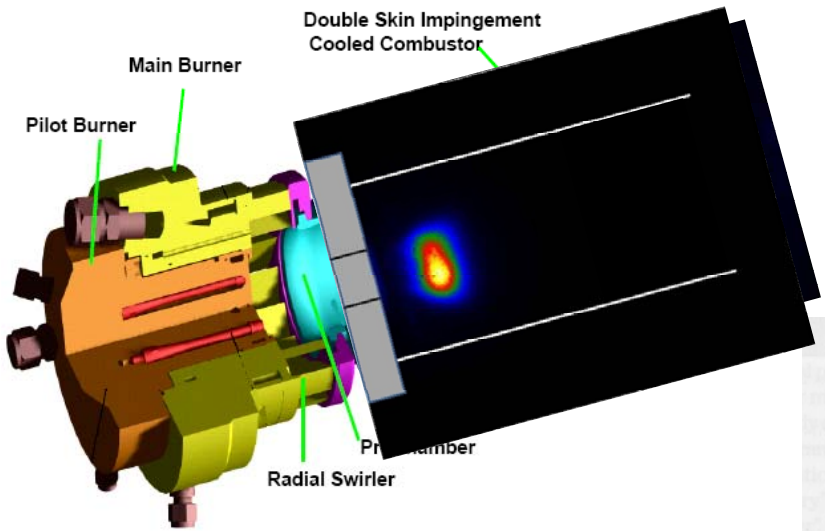
# Key Questions: Operability

- **Key Operability Concerns**
  - **Static Stability (Blow off limits)**
  - **Flashback**
  - **Autoignition**
  - **Combustion Dynamics**

- **Examples**

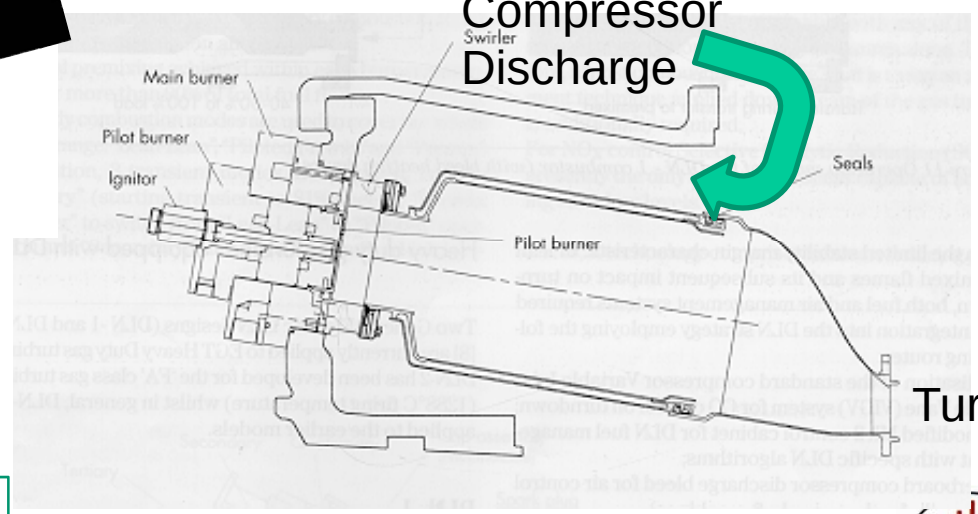
# Flashback

- **Consider use of syngas in advanced lean premixed combustor optimized for natural gas**




OH* visualization (Heat release marker)
Reaction Structure
$T_{ad}$ = 1780 deg-K

Substantially different reaction structure for different fuels with same firing temperature

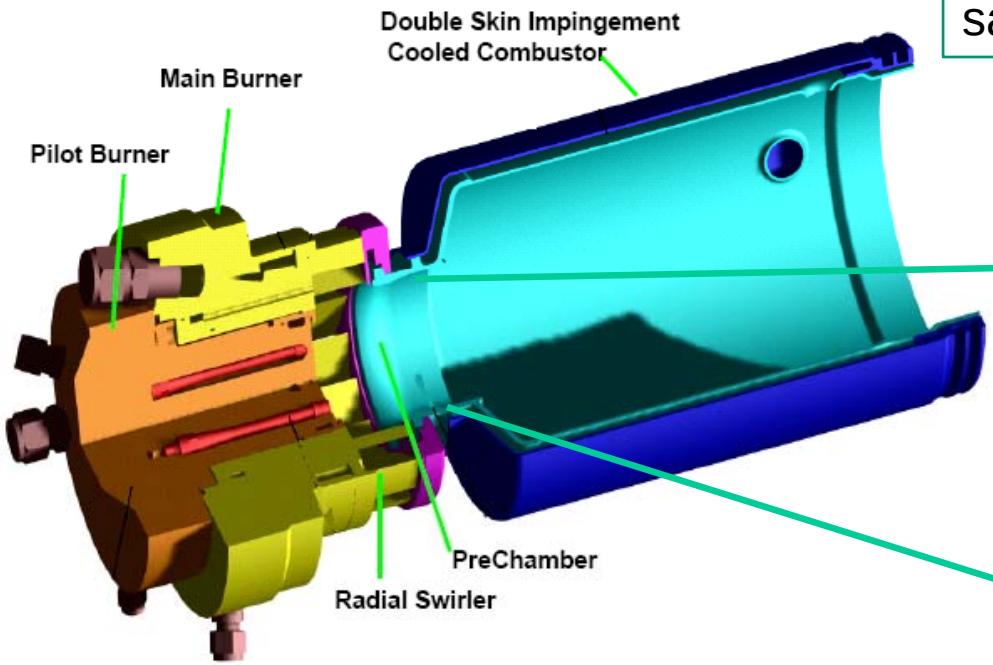



Ignition, heat release, flame speed

# Flashback

- **Consider use of syngas in advanced lean premixed combustor optimized for natural gas**

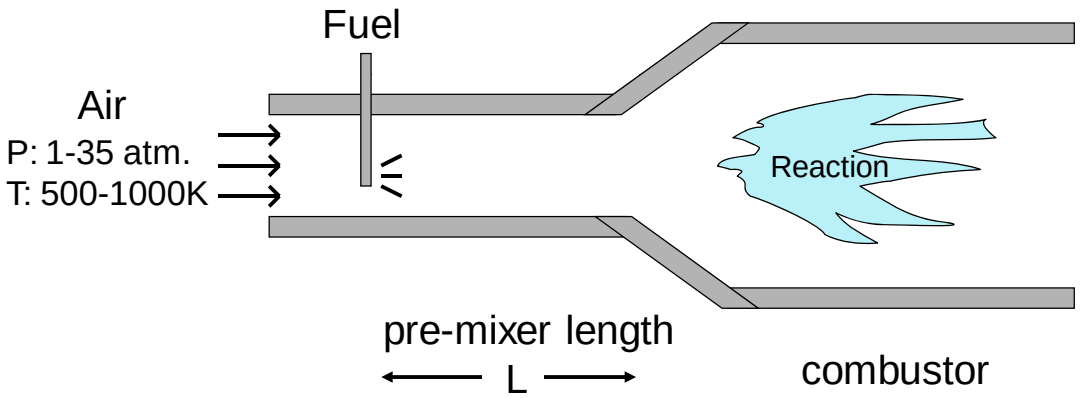
Substantially different flame speed for different fuels with same firing temperature



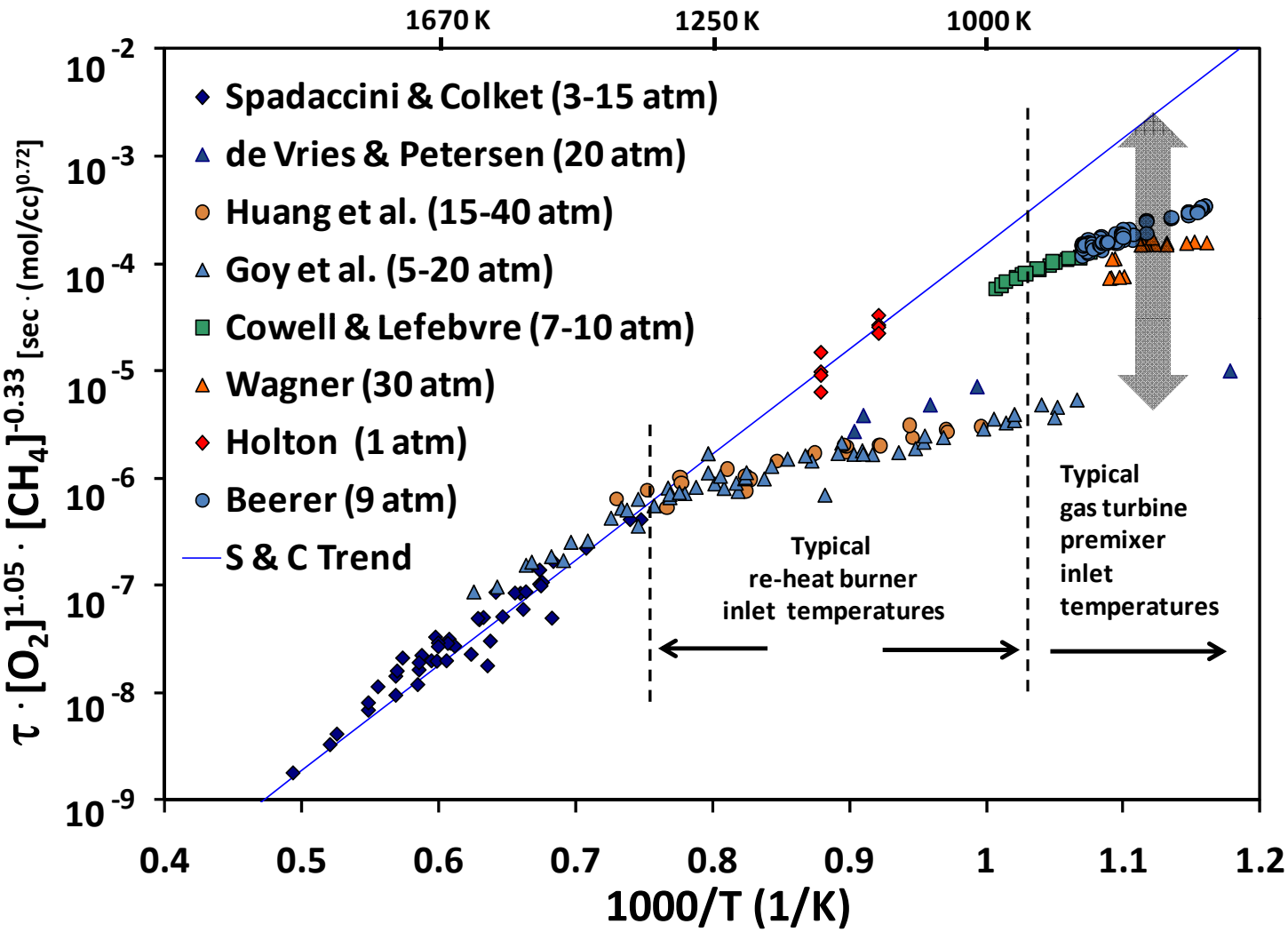
Flashback or autoignition w/high hydrogen content fuel damaged prechamber

Prediction of ignition behavior and flame speed critical

# Autoignition

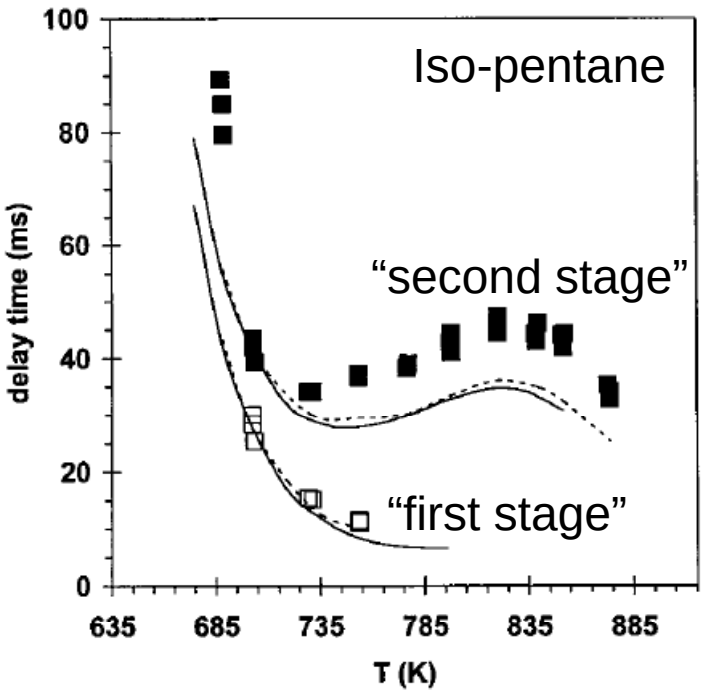


# Autoignition



# Autoignition

- **Negative Coefficient Region**
  - **Can result in shorter delay times at even cooler temperatures**
    - **Some focus for recip applications**
    - **Not commonly looked at for pure fuels, typical nat gas compounds used for gas fired systems**
    - **Relevant for C3+**
    - **Isomers will behave differently (iso vs n)**
    - **Typified by early reactions (generally non-homogenous behavior) and later reactions (more homogeneous)**
    - **Similar behavior observed for hydrogen**

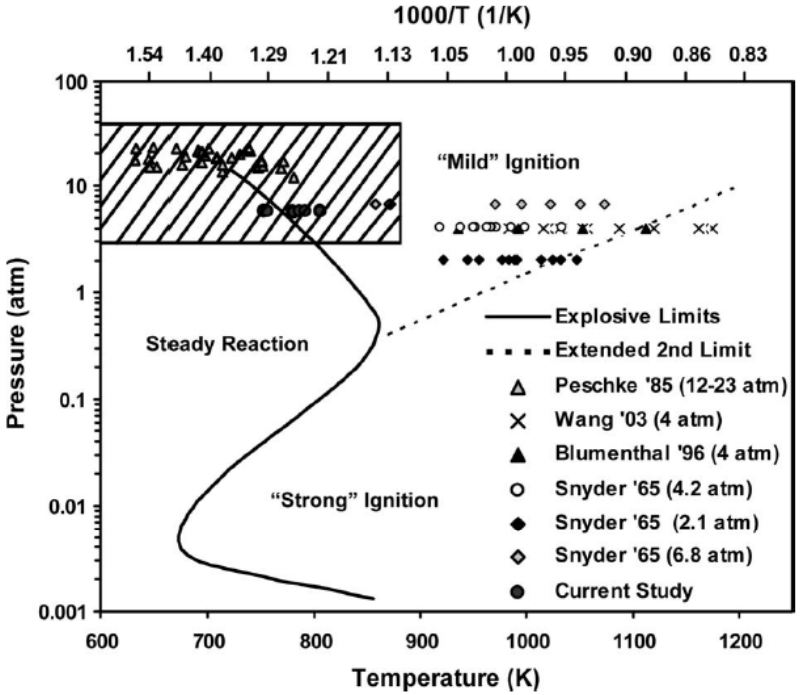


(a)

Ribacour, et al., 2000

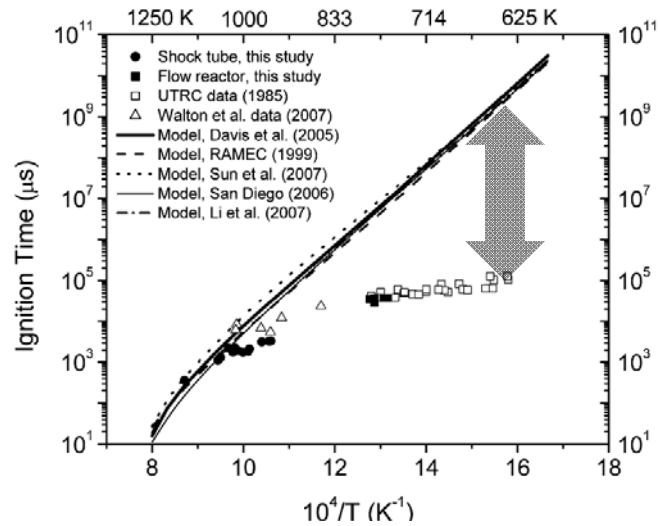
# Autoignition

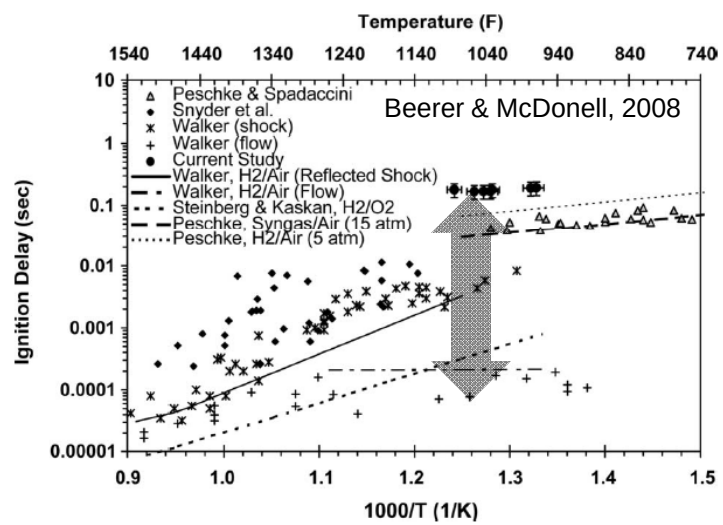
- **High hydrogen content fuels….**




Beerer & McDonell, 2008

E.L. Petersen et al. / Combustion and Flame 149 (2007) 244–247



# Key Questions: Operability

- **Key Physics**
  - **Static Stability (Blow off limits)**
    - **Kinetics of reaction (fuel dependent), aerodynamics of flow**
  - **Flashback**
    - **Flame speed/propagation (fuel dependent), aerodynamics of flow in premixer**
  - **Autoignition**
    - **Kinetics of early reactions (fuel dependent), residence times/flow in premixer**
  - **Combustion Dynamics**
    - **Kinetics of reaction (fuel dependent), relation between flame position and heat release location (fuel dependent), acoustic properties of geometry**
- **Insufficient data available for alternative fuels at conditions for practical devices**

# Key Questions: Emissions

- **Emissions Questions and Key Physics**
  - **NOx, while traditionally controlled with reducing temperature, is also formed through other pathways ($N_2O$, NNH, Prompt, etc.)**
    - **The details of these paths still being understood**

- **Insufficient data available for conditions and fuels of interest**

# Required

- **Detailed data to support advanced analysis and model development**
  - **Ignition delay**
  - **Flame speed (turbulent as well as laminar)**
  - **Evaluation of chemistry**

- **Assimilation of data into interchange criteria**
  - **Consider existing starting points (generally 1-D type)**
  - **Consider more sophisticated 2 or 3D strategies (e.g., reactor networks)**

- **Evaluation of interchange criteria**
  - **Existing model combustors, turbines, engines**

# Research Team

- **Vince McDonell, UC Irvine**
  - **David Beerer**
  - **Zhixuan Duan**
  - **Joe Velasco**

- **Tim Lieuwen, Georgia Institute of Technology**
  - **Andrew Marshall**
  - **Bobby Noble**

- **Phil Malte/John Kramlich, University of Washington**
  - **Igor Novosselov**
  - **Boyd Fackler**
  - **Megan Karalus**

# Project Tasks

- **Task 1—Administration**
  - **Project Advisors**
- **Task 2—Coordination & GFIC Development**
- **Task 3—Chemical Mechanism Work (UW)**
- **Task 4—Ignition/Flashback/Blowoff Work (UCI)**
- **Task 5—Turbulent Flame Speed Work (GT)**

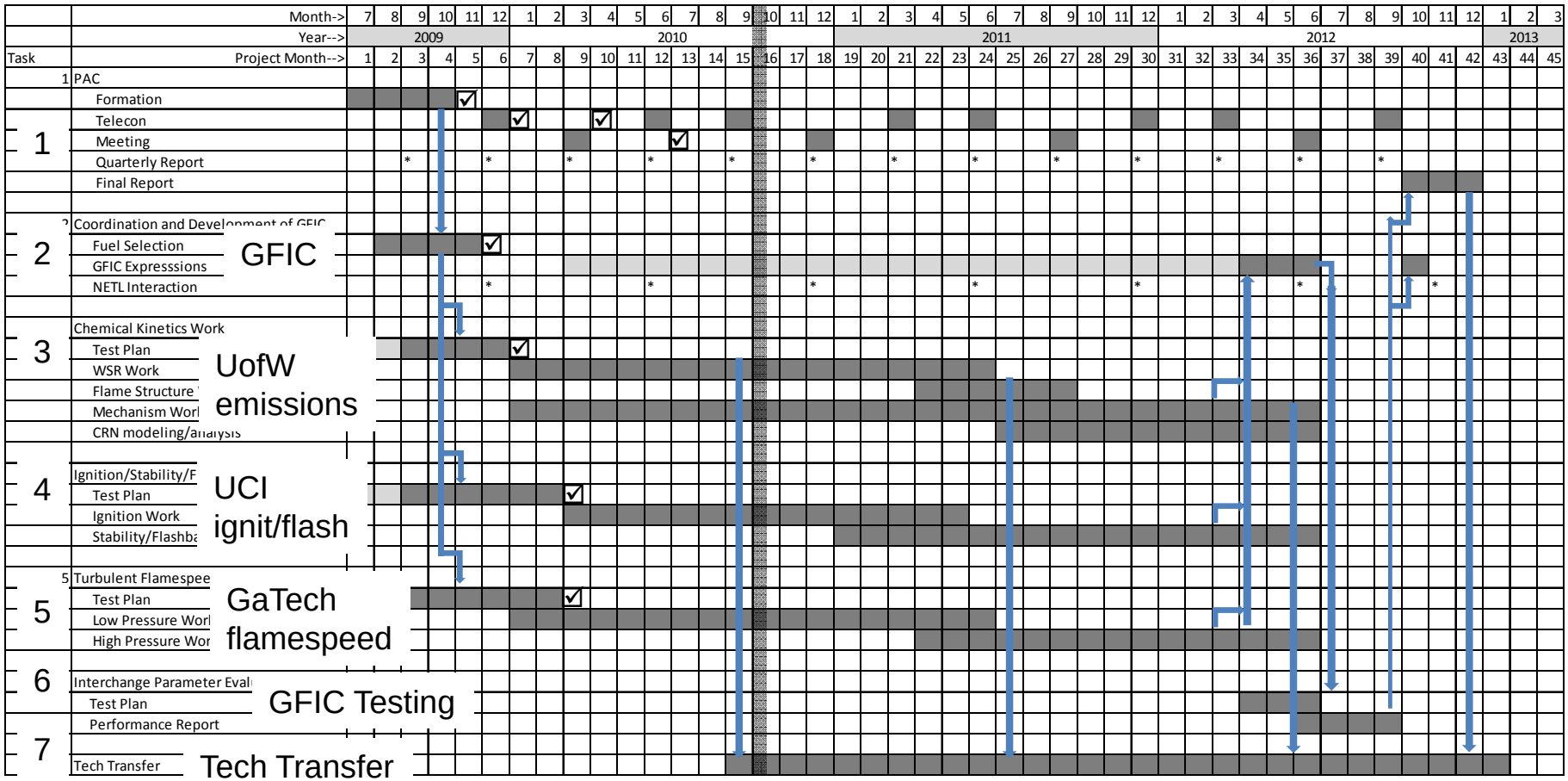
3 years
>80% of
effort

- **Task 6—Interchange Parameter Testing**

- **Task 7—Technology Transfer**

# Project Tasks

- **Current Status**

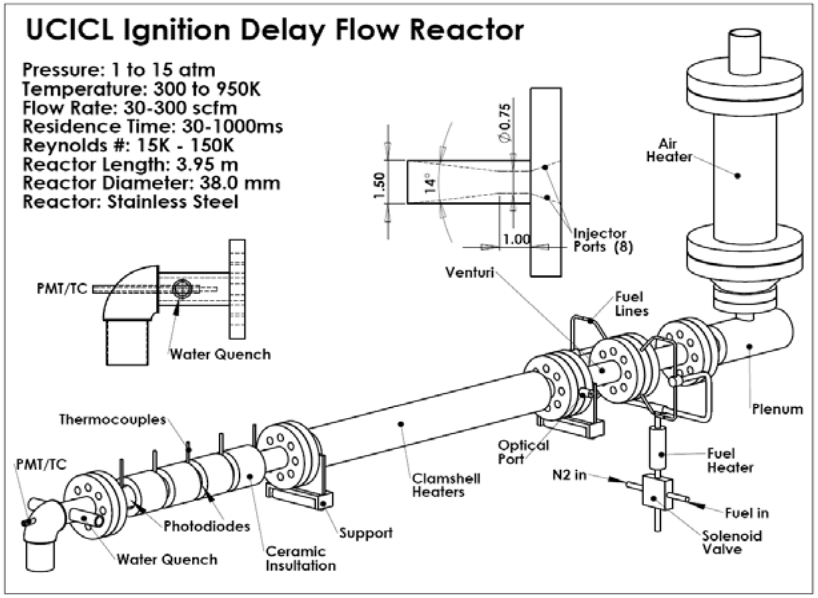


# Fuel Selection

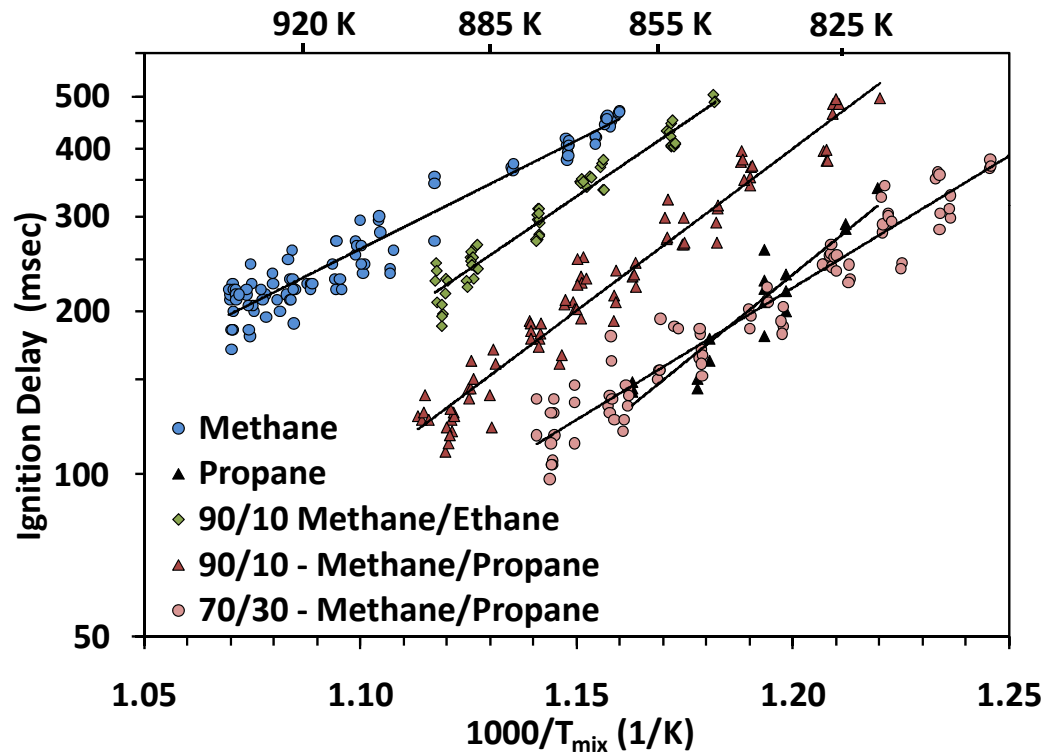
- **Consensus Fuels / Compositional Ranges**

| Source | H2 | CO | CH4 | CO2 | N2 | C2 | C3 |
|---|---|---|---|---|---|---|---|
| High H2 | 90- 100 | 0 - 10 | | | | | |
| Process and Refinery Gas | 25 - 55 | 0 - 10 | 30 - 65 | 0 - 5 | | 0 - 25 | 0 - 25 |
| Gasified Coal/Petcoke (O2 Blown) | 35 - 40 | 45 - 50 | 0 - 1 | 10 - 15 | 0 - 2 | | |
| Gasified Biomass (air blown) & Gasification w/ N2 Dilution | 15 - 25 | 15 - 35 | 0 - 5 | 5 - 15 | 30 - 50 | | |
| Landfill / Digester | | | 35 - 65 | 35 - 55 | 0 - 20 | | |
| LNG | | | 86- 97 | | 0 - 3 | 2 - 11 | 0 - 2 |
| Shale Gas | | | 82-97 | 0-3 | | 0 - 14 | 0 - 1 |
| Associated Gases | | | 75- 95 | | | 5 - 25 | |

# Example Result: Ignition Delay



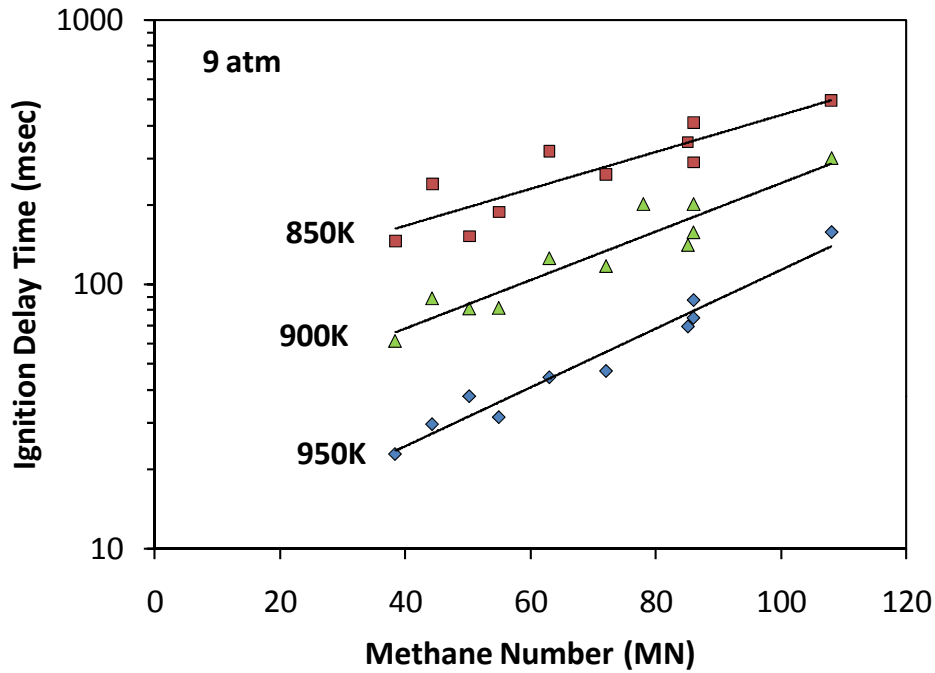

| | H2 | CO | CH4 | CO2 | N2 | C2 | C3 |
|---|---|---|---|---|---|---|---|
| Pure Fuels | 100 | | | | | | |
| | | | 100 | | | | |
| | | | | | | 100 | |
| | | | | | | | 100 |
| Landfill and Digester Gas | | | 75 | 25 | | | |
| | | | 50 | 50 | | | |
| | | | 50 | | 50 | | |
| Process and Refinery Gas | 10 | | 90 | | | | |
| | 20 | | 80 | | | | |
| | 40 | | 60 | | | | |
| | 60 | | 40 | | | | |
| | 25 | | 50 | | | 25 | |
| Gasification Fuels | 45 | 45 | 10 | | | | |
| | 30 | 60 | 10 | | | | |
| Gases LNG/Shale/Associated | | | 90 | | | 10 | |
| | | | 85 | | | 15 | |
| | | | 70 | | | 30 | |
| | | | 95 | | | | 5 |
| | | | 90 | | | | 10 |
| | | | 70 | | | | 30 |
| | | | 70 | | | 15 | 15 |



# Example Result: Ignition Delay

- **Analysis of Ignition results for alkanes**
  - **Correlation with MN➔**
  - **Design guides ➓**

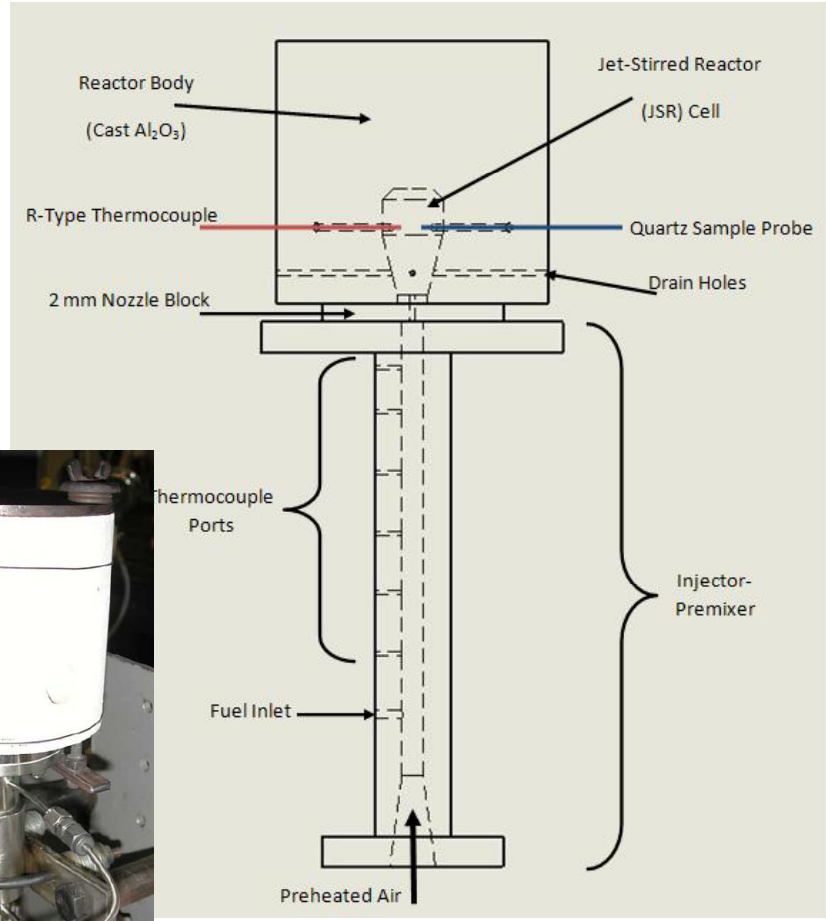
| Fuel | Composition | Ignition Delay Expression |
|---|---|---|
| 1 | Methane | $\tau = 9.08 \times 10^{-5} \cdot \exp\left(\frac{18.425}{RT}\right) P^{-1.0}$ |
| 2 | Ethane | $\tau = 5.71 \times 10^{-9} \cdot \exp\left(\frac{33.540}{RT}\right) P^{-1.0}$ |
| 3 | Propane | $\tau = 3.29 \times 10^{-8} \cdot \exp\left(\frac{29.765}{RT}\right) P^{-1.0}$ |
| 4 | 90% Methane, 10% Ethane | $\tau = 1.66 \times 10^{-6} \cdot \exp\left(\frac{24.865}{RT}\right) P^{-1.0}$ |
| 5 | 85% Methane, 15% Ethane | $\tau = 1.19 \times 10^{-6} \cdot \exp\left(\frac{25.410}{RT}\right) P^{-1.0}$ |
| 6 | 70% Methane, 30% Ethane | $\tau = 2.41 \times 10^{-8} \cdot \exp\left(\frac{31.590}{RT}\right) P^{-1.0}$ |
| 7 | 95 % Methane, 5% Propane | $\tau = 7.41 \times 10^{-6} \cdot \exp\left(\frac{21.750}{RT}\right) P^{-1.0}$ |
| 8 | 90 % Methane, 10% Propane | $\tau = 2.30 \times 10^{-7} \cdot \exp\left(\frac{27.435}{RT}\right) P^{-1.0}$ |
| 9 | 70 % Methane, 30% Propane | $\tau = 2.76 \times 10^{-6} \cdot \exp\left(\frac{22.330}{RT}\right) P^{-1.0}$ |
| 10 | 70% Methane, 15% Ethane, 15% Propane | $\tau = 8.05 \times 10^{-8} \cdot \exp\left(\frac{28.660}{RT}\right) P^{-1.0}$ |
| 11 | Simulated Natural Gas | $\tau = 1.15 \times 10^{-8} \cdot \exp\left(\frac{33.120}{RT}\right) P^{-1.0}$ |
| 12 | Irvine Natural Gas | $\tau = 7.44 \times 10^{-7} \cdot \exp\left(\frac{25.750}{RT_{mix}}\right) P^{-1.0}$ |



# Example Results: Emissions

- **UofW Jet Stirred Reactor**
  - **Residence Time: 2 – 3 ms**
  - **Temperature: 1800 K**
  - **Da: 0.1 – 1.5 in the RZ**

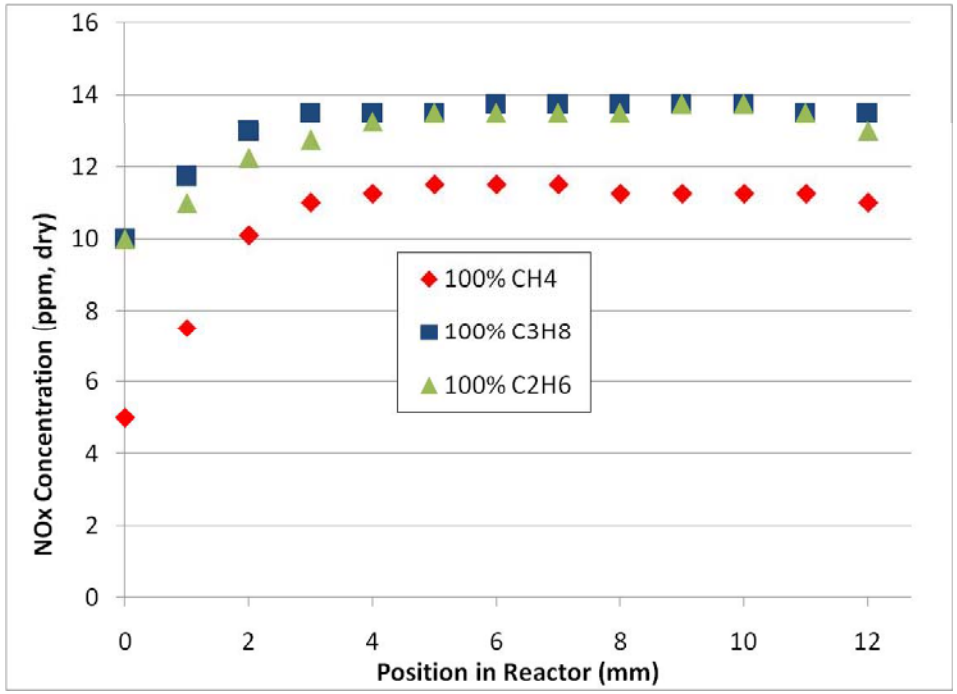
| Mixture | Source | | $H_2$ | CO | $CH_4$ | $CO_2$ | $N_2$ | $C_2$ | $C_3$ |
|---|---|---|---|---|---|---|---|---|---|
| 1 | High $H_2$ | Range in Field | 90-100 | 0 - 10 | | | | | |
| | | Nominal Fuel | 100 | | | | | | |
| | | Alternative Fuel | 90 | 10 | | | | | |
| 2 | Process and Refinery Gas | Range in Field | 25 -55 | 10 | 30 - 65 | 5 | | 0-25 | 0-25 |
| | | Nominal Fuel | 25 | | 50 | | | 25 | |
| | | Alternative Fuel 1 | 25 | | 50 | | | | 25 |
| | | Alternative Fuel 2 | 25 | | 65 | | | 10 | |
| | | Alternative Fuel 3 | 55 | | 35 | | | 10 | |
| 3 | Gasified Coal/Petcoke ($O_2$ Blown) | Range in Field | 35 - 40 | 45- 50 | | 10 - 15 | | | |
| | | Nominal Fuel | 40 | 50 | | 10 | | | |
| | | No Alternatives | | | | | | | |
| 4 | Landfill & Digester Gas | Range in Field | | | 35 - 65 | 35 - 55 | 0 - 20 | | |
| | | Nominal Fuel | | | 50 | 35 | 15 | | |
| | | Alternative Fuel 1 | | | 50 | 50 | | | |
| | | Alternative Fuel 2 | | | 50 | | 50 | | |
| 5 | LNG | Range See below | | | 75- 95 | | | 5 - 25 | |
| | Shale Gas | Range See below | | | 82 - 97 | 2.5 | | 0 - 14 | 1 |
| | Associated Gas | Range See below | | | 75- 95 | | | 5 - 25 | |
| | LNG/Shale/ Associated Gases | Nominal Fuel | | | 95 | | | 5 | |
| | | Alternative Fuel 1 | | | 90 | | | 10 | |
| | | Alternative Fuel 2 | | | 75 | | | 25 | |
| | | Alterntative Fuel 3 | | | 75 | | | | 25 |



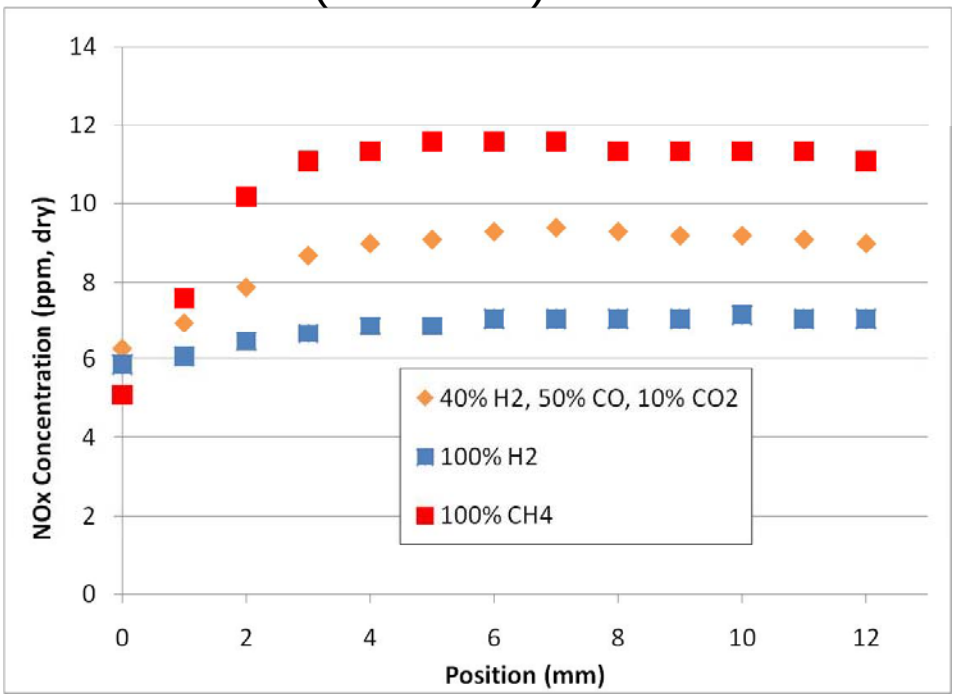
# Example Results: Emissions

- **Emissions Observations (fixed residence time, fixed reaction temperature)**

Pure Alkanes

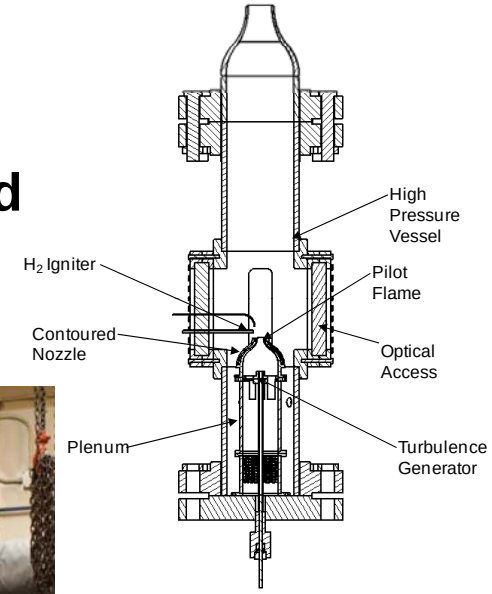



Gasified Coal (O2 blown)



# Summary

- **The research teams are making steady progress relative to data gathering**
  - **UCI: Ignition Delay**
  - **GaTech: Laminar and Turbulent Flame Speed**
  - **UCI: Flashback**
  - **UofW: Emissions, Blowoff**

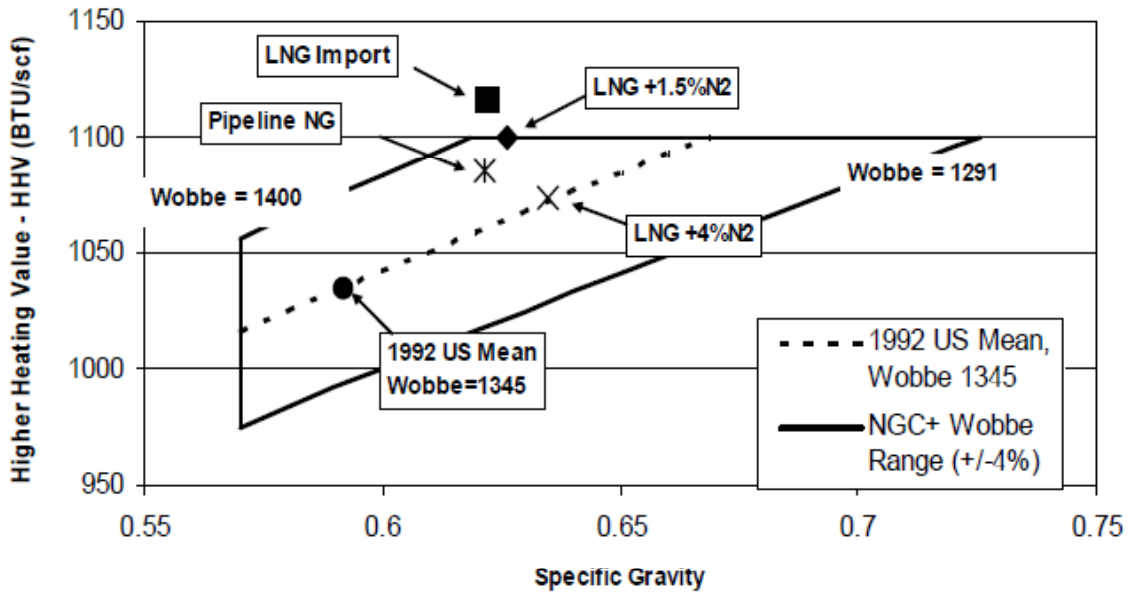



- **Data analysis initiated**
  - **Correlation development**
  - **Mechanism evaluation**
  - **Legacy interchange parameters gathered**

# Interchange Parameters

- **Wobbe Index**

$$WI = \frac{HHV}{\sqrt{S.G.}}$$




  - **Most widely used parameter—associated with volumetric throughput**
  - **Really a supply/fuel system parameter**
  - **Used in recent LNG discussions**

$$MWI = \frac{LHV}{\sqrt{T}\sqrt{S.G._{fuelvsair,\ ISO}}}$$

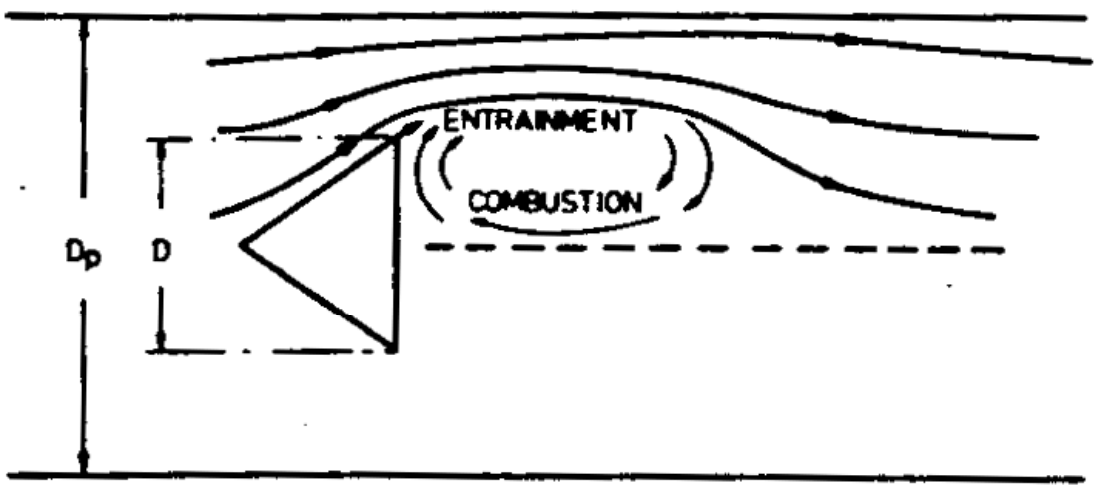
  - **MWI—tailor using fuel temperature (GE OpFlex™)**

# Interchange Parameters

- **Methane/Cetane Numbers**
  - **Analogous to "Octane Rating"--a measure of resistance to autoignition of the gaseous fuel (i.e., "knock")**
  - **Methane Number**
    - **Used in the context of CNG vehicles**
      - Used to set fuel standard (e.g., MN = 85)
      - Hydrogen = 0
      - Methane = 100
  - **Cetane Number**
    - **Used for compression ignition applications (higher means easier to ignite—good for high speed engines)**

# Interchange Parameters

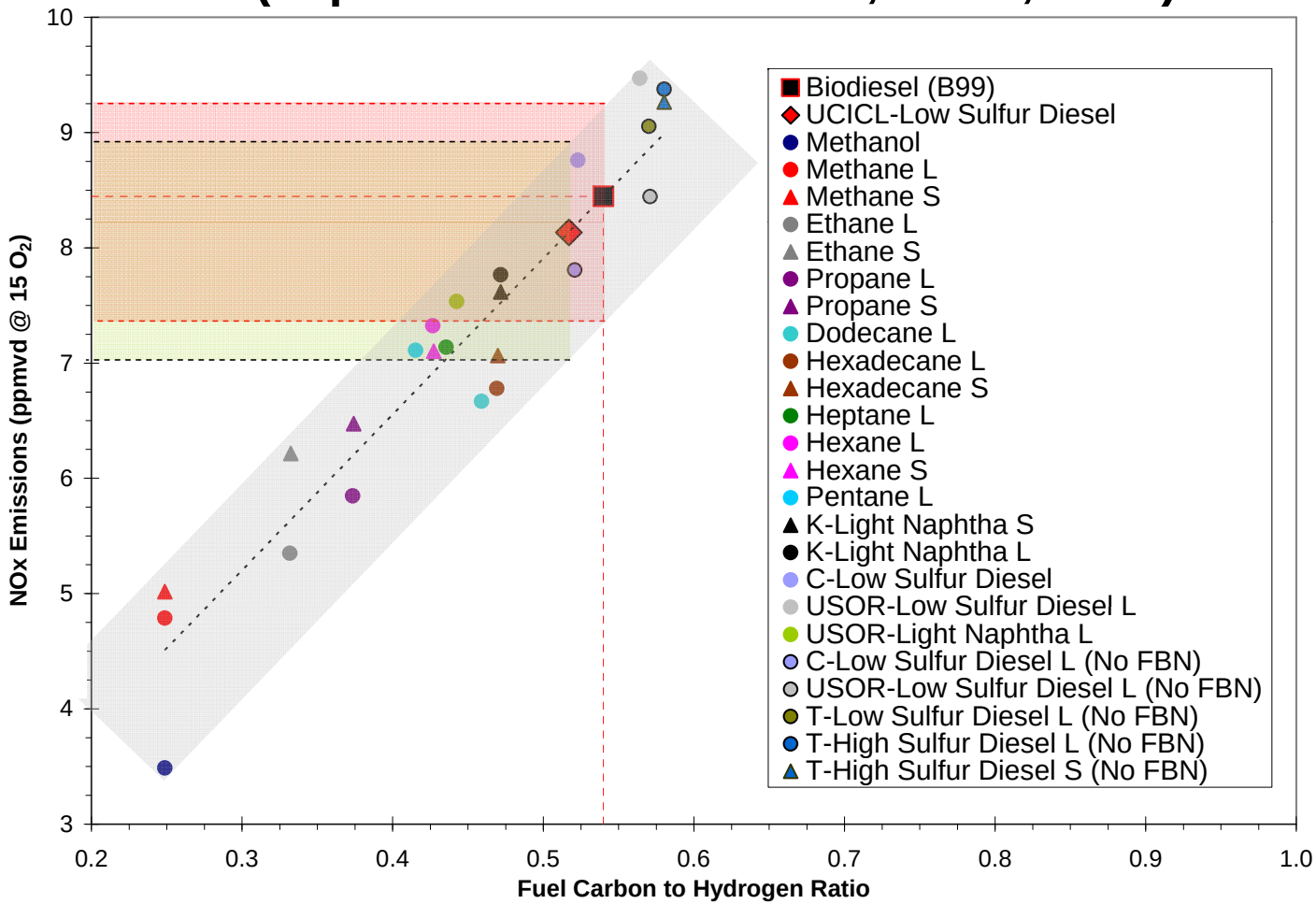
- **Stability (example)—spring board for flashback?**
  - **Lefebvre**
    - **Competition between heat release rate and residence time (Da)**




$$q_{LBO} = C\left[\frac{\dot{m}_A}{V_c P_3^{1.25} \exp\left(T_3/150\right)}\right]^{0.16}$$

# Interchange Parameters

- **Emissions example**
  - **C:H ratio (adpated from UofW—Lee, Malte, et al.)**



# Interchange Parameters

- **Emissions example**
  - **Lefebvre "Severity Parameter"**

$$S_{NOx} = \left(\frac{P_3}{432.7}\right)^{0.4} e^{\left(\frac{T_3 - 1027.6}{349.9} + \frac{6.29 - Ho}{53.2}\right)}$$

$P_3$ = Combustor inlet pressure (psia)

$T_3$ = Combustor inlet temperature (°F)

Ho = Ambient air humidity (g/kg air)

  - **Fixed Fuel!**
  - **Unclear if applicable to lean burn systems**