Energy Conversion and Combustion Sciences

08 MAR 2012

Chiping Li
Program Manager
AFOSR/RSA
Air Force Research Laboratory

Integrity ★ Service ★ Excellence

Report Documentation Page

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NAME: **Chiping Li**

BRIEF DESCRIPTION OF PORTFOLIO:

Objectives:

- Understand ***Combustion Fundamentals***
- Quantify ***Rate Controlling Processes and Scales***

Scope:

- key multi-physics and multi-scale phenomena in combustion processes
- ***Interests to the Air Force*** propulsion applications.
- All aspects related to the above with the ***following emphasized Sub-Areas:***

LIST SUB-AREAS IN PORTFOLIO:

1. Combustion Diagnostics

2. Turbulence Combustion Experiments

3. Combustion Modeling and Theory

4. Innovative Chemical-to-Mechanical Energy Conversion/Combustion Processes

Note: The above sub-areas will be further discussed on the following pages.

New Portfolio Emphases

Based on the solid foundation built by Dr. Julian Tishkoff, the new portfolio focuses more on:

- ***Combustions Fundamentals;***
- ***Ab Initio Modeling;***
- ***Air Force Relevant Conditions.***

Emphasized sub-areas:

1. Advance of diagnostics **(continuous investments)**:
   - Enabling tools to observe the nature and obtain data
2. Well Designed Experiments to **(new focus)**:
   - Understanding key combustion phenomena and characteristics
   - Identifying and quantifying rate-controlling processes
   - At ***compressible, High-Re conditions*** relevant to AF propulsion system, e.g. turbine ram/scramjet, and rocket engines
3. Combustion Modeling and Theory **(new focus with some existing elements)**:
   - ***Ab Initio*** and data-based Combustion-Chemistry and turbulence combustion
   - Numerical experiments
4. Innovative Energy Conversion/Combustion Processes **(new focus with some existing elements):**
   - Potential game changing concepts
   - Injecting rate-controlling factors if necessary

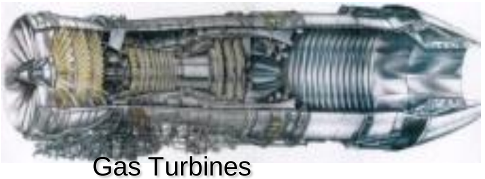
Key Combustion Phenomenon

Turbulent combustion – the key Combustion phenomenon in most of AF propulsion systems:

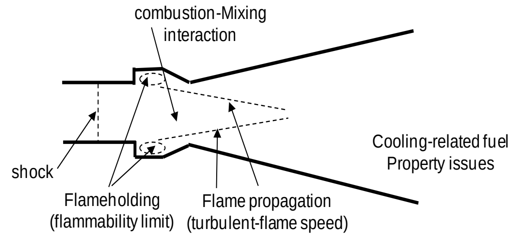
- One of ***most important*** determining factors of operability and performance;
- One of ***least understood*** areas in basic combustion research, with large uncertainties;
- Confluence of a "grand-old" fundamental science problem, immediate needs and long-term interests;
- Recent advances in diagnostics resulted from persistent investments by Dr. Julian Tishkoff provided needed experiment toots.


Rockets

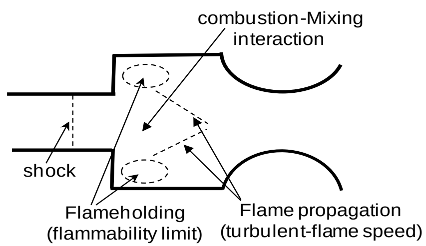

Hypersonics


Gas Turbines

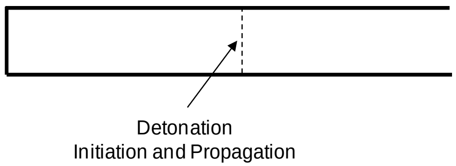
Cavity Based Scramjet Combustor

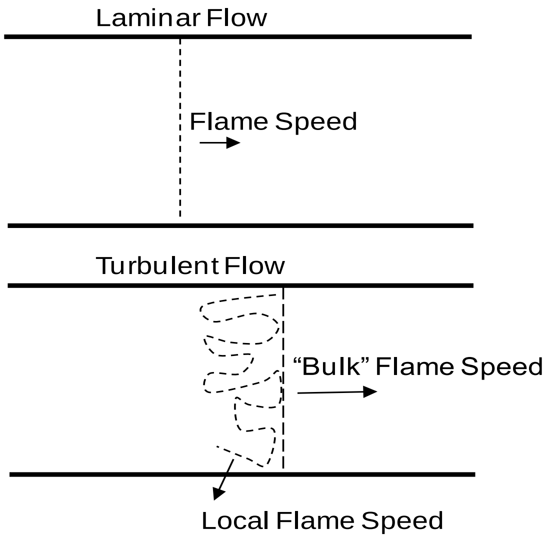


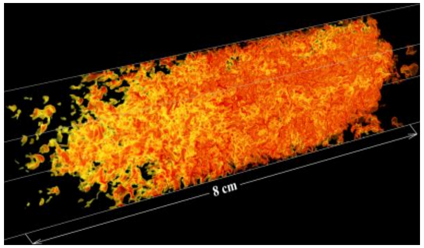
Ramjet Dump Combustor



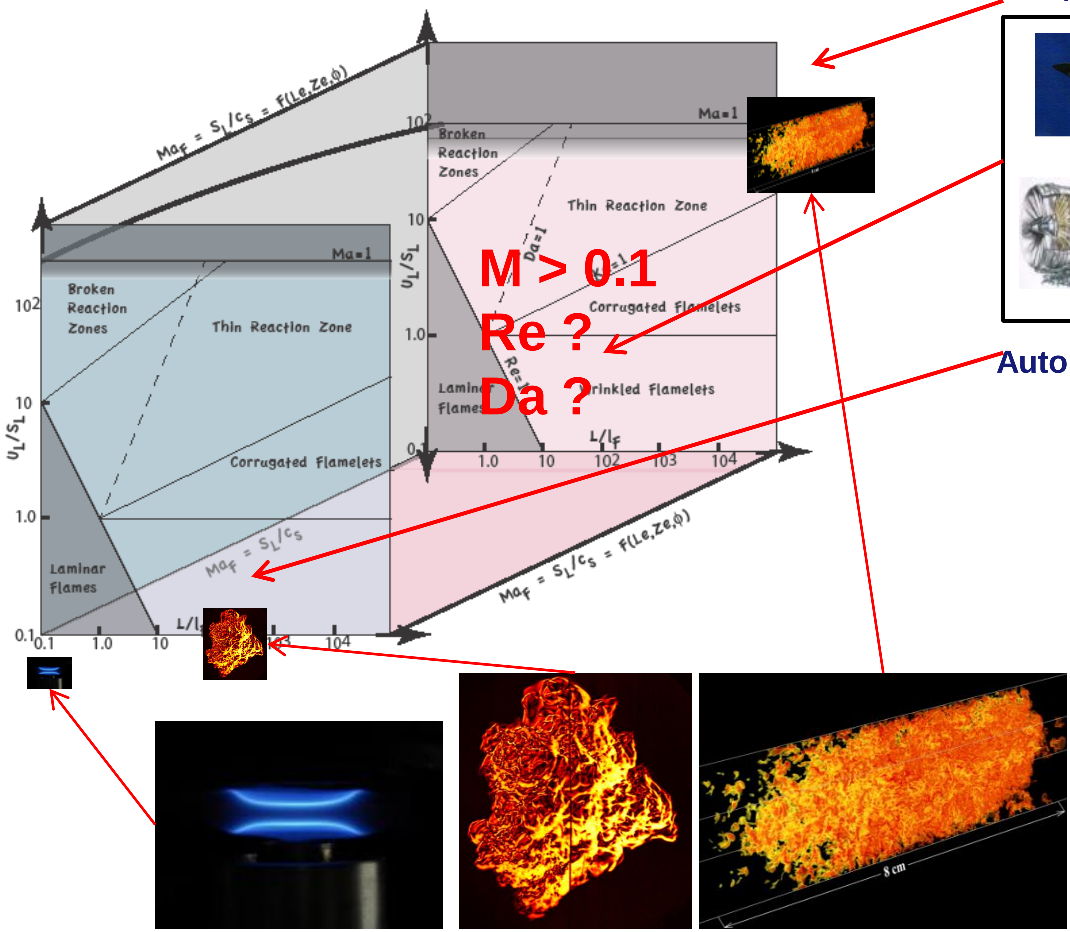
Pulse Detonation Engine



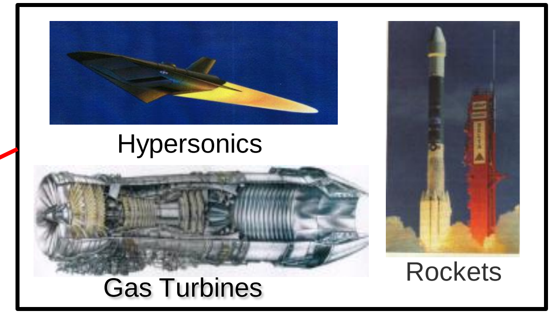




Turbulence Combustion: Fundamental Structures, Critical Scales and Relevant Conditions



laminar flame L-M, L-Re (wrangled flame) Hi-M, Hi-Re (small



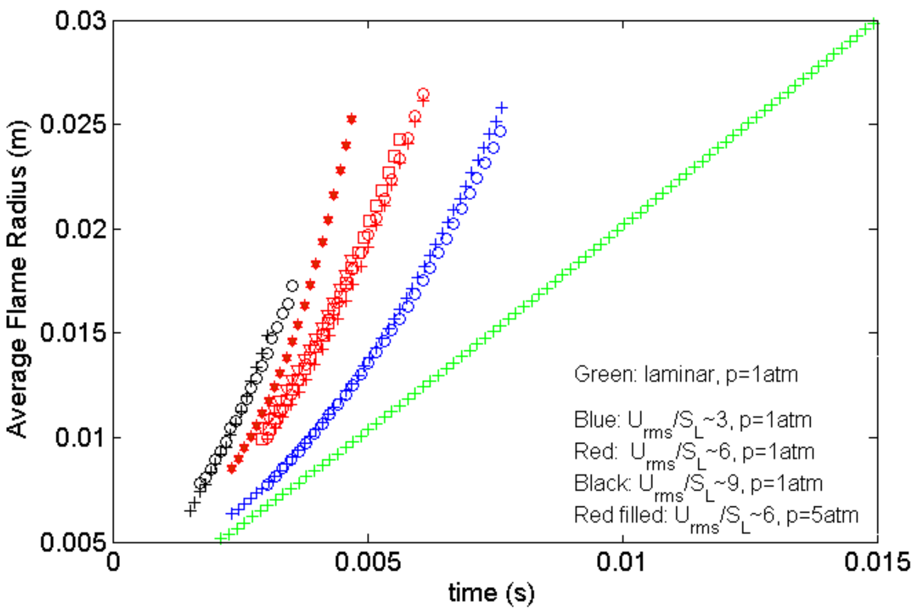
Key Observation:
Little data available at compressible , High-Re conditions.

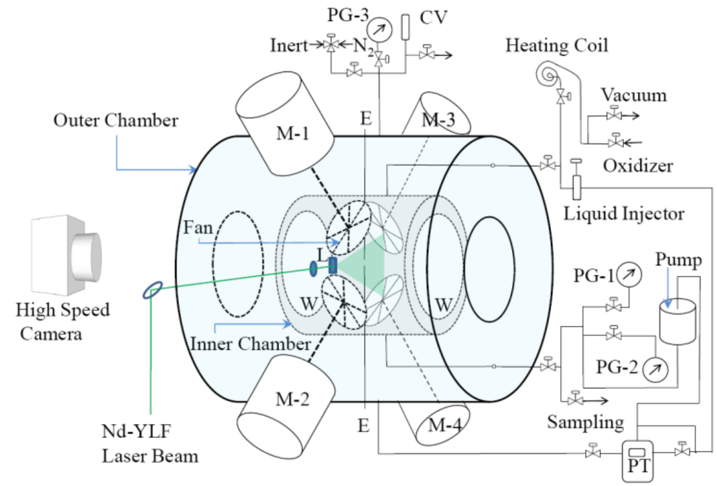
Key Questions:
•*Flame Structure?*
•*Regime Boundaries?*
•*Critical Scales?*
•*Relevant Conditions?*
•*Rate-Controlling Processes?*

(1)Little Data Available at Compressible, High-Re Conditions;
(2)Needs for Better Definition of Re-Conditions in Regions of Interests

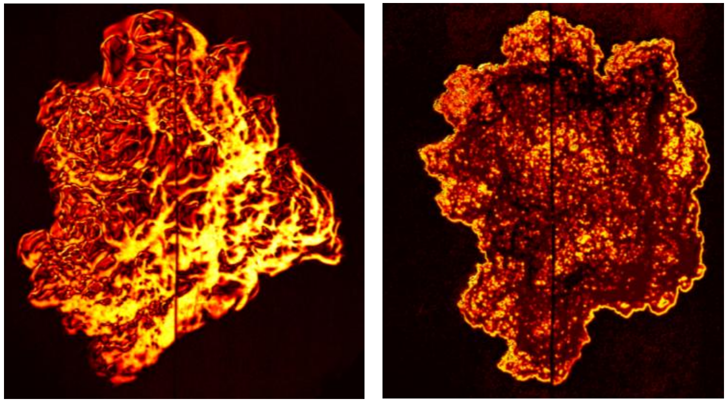
Low-Re Bounding Experiment (Physical)

Flame Speed and Self-similar Propagation of Turbulent Premixed Flames: (PI: Law, Princeton)





CV: Check Valve, PG: Pressure Gauge, PT: Pressure Transducer, M: Fan Motor, L: Cylindrical Lens, E: Electrodes, W: Quartz Window



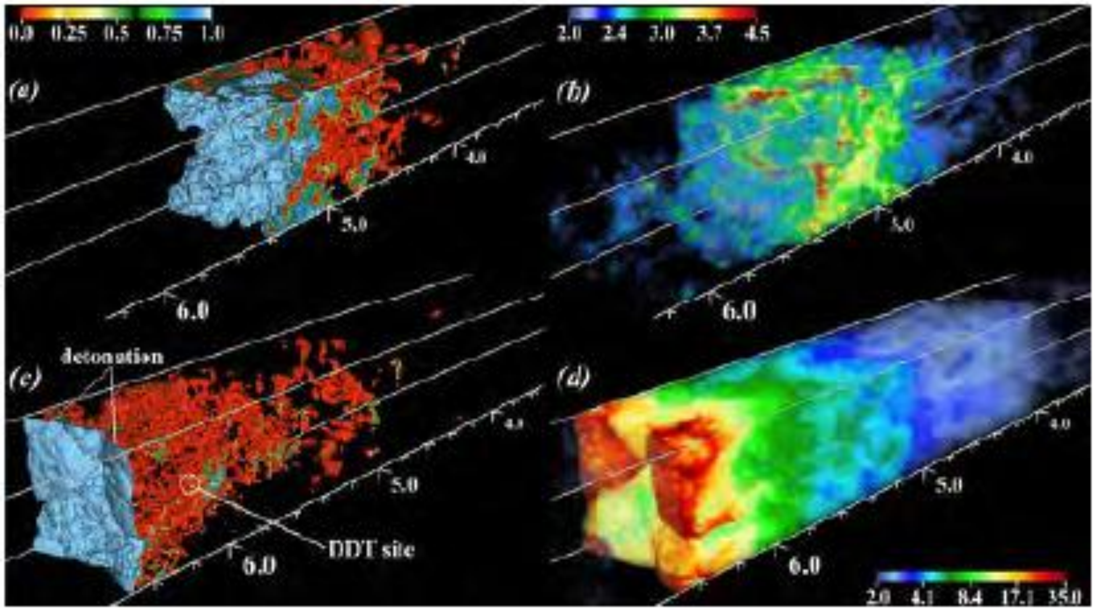
Pressure = 1atm Pressure = 5atm

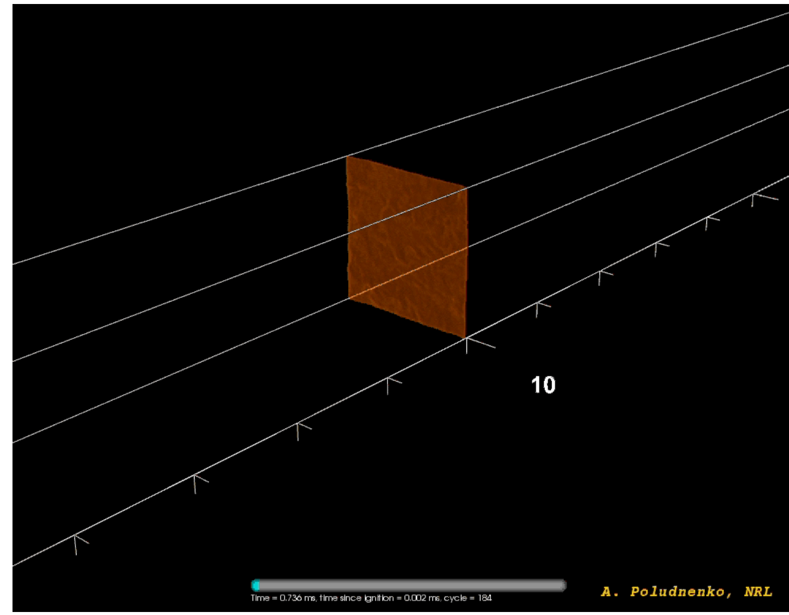
Schlieren images of turbulent premixed CH_4-air flames (ϕ=0.9, *Le*=1) at same u_{rms}

Turbulence Already Affects Flame Structure and Speed at Relatively Low Re Conditions

High-Re Bounding Experiment (Numerical)

Non-equilibrium, Non-Kolmogorov Turbulence in High-Speed Combustion Flows:
(PI: Oran, MIPR-NRL)





At High-M, High-Re Conditions, Turbulence Significantly Increases Flame Surface and Global Burning Speed.
(If the criterion on the right is satisfied, DDT starts.)

$$S_T = \frac{c_s}{(\rho_f/\rho_p)}$$

Multi-Physics and Multi-Scale Nature of Turbulence Combustion

Turbulence combustion:

- Quintessentially multi-physics and multi-scale
- Many interacting processes and scales
- Multiple numerical issues involving many disciplines in mathematics

1. **Intersection of two highly nonlinear processes – Turbulence & Combustion Chemistry**
   - Energy release to the flow during combustion
   - Compressibility and strong Pressure (shock & expansion) waves

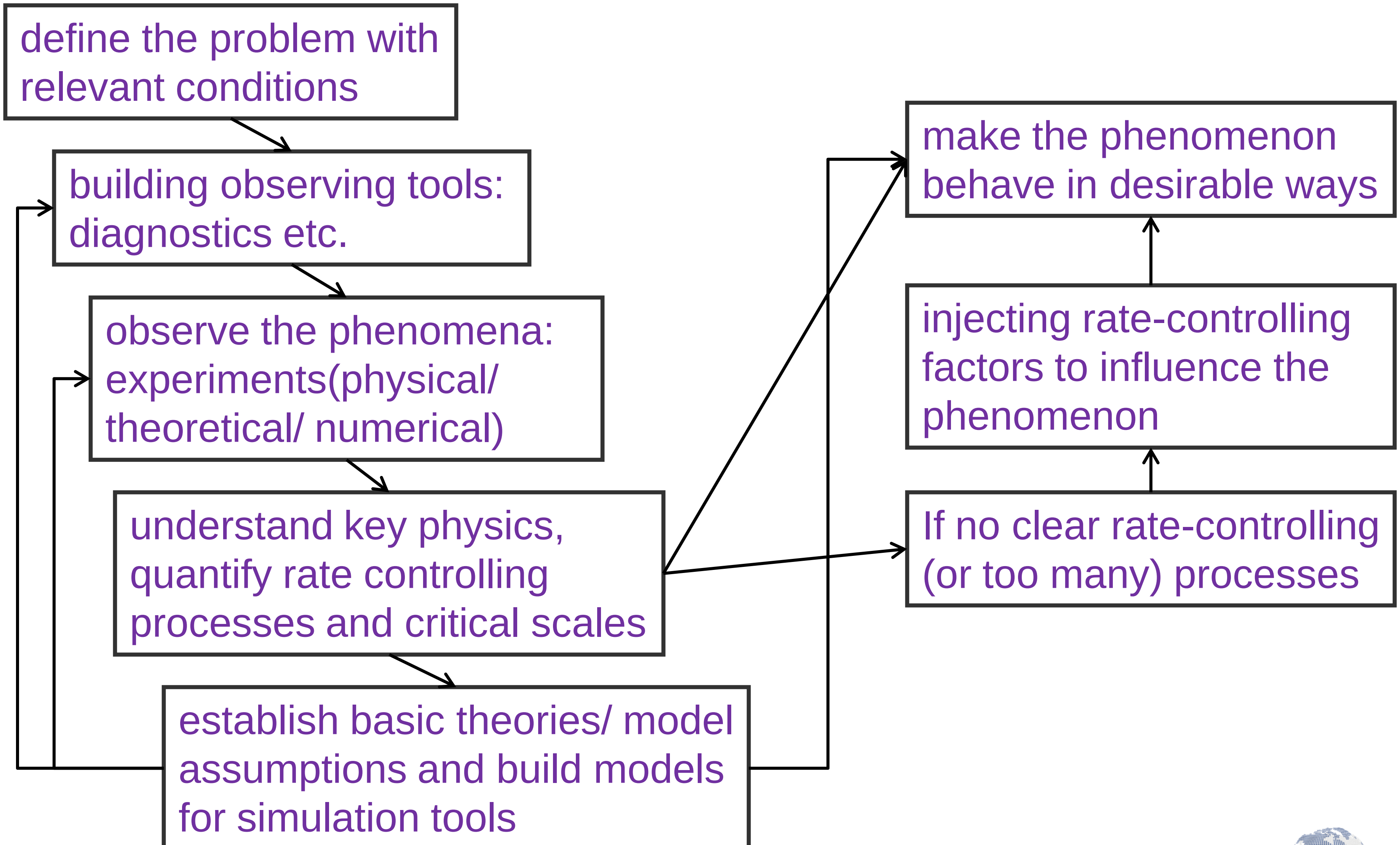
2. **Energy Transport Process**
   - Diffusion
   - Conduction
   - Radiation
   - Internal Molecular Energy Transfer (thermally non-equilibrium)

3. **Multi-Phase Interactions**
   - Multi-phase combustion (e.g. spray injection/combustion)
   - Interaction with solid-state surface (e.g. coking)

4. **Numerical and Mathematical Issues**
   - Initial and Boundary conditions
   - Numerical stabilities

Multi-Disciplinary Collaboration is Essential to the Success

An Effective Approach Dealing with Multi-Physics and Multi-Scale Phenomena



Coordination with Other Agencies

1. **Strong collaboration is continuously being forged in following areas:**
   - Diagnostics (Mainly DoE, NASA)
   - Numerical (DoE, NASA, ARO)
   - Combustion Chemistry (DoE, ARO, NSF)
   - Innovative Combustion Concept (ONR, ARO)

2. **Dividing problems and condition areas according to each interests:**
   - AFOSR combustion portfolio -- in turbulence combustion area:
     - Air-Force relevant conditions, i.e.:
     - Compressible and high-Re conditions for propulsion applications
   - DOE -- a well funded combustion program focusing on basic energy research – in turbulence combustion area:
     - Ground-base energy systems and auto-engine types of applications
     - Relatively low-speed and low-Re conditions (TNF etc.)
   - NASA -- a modest combustion program focusing:
     - "Very-high" speed (space access) region
     - Overlapping interests and close coordination with AF programs (scramjet, rockets etc.).
   - NSF -- a modest combustion program:
     - Covers broad ranges of combustion problems

3. **Multi-Agency Coordinate Committee of Combustion Research (MACCCR)**
   - Functioning well and its positive role will continue

Multi-Agency Collaboration Benefits Every One

Combustion Diagnostics

Enabling tools to observe the nature and obtain data:

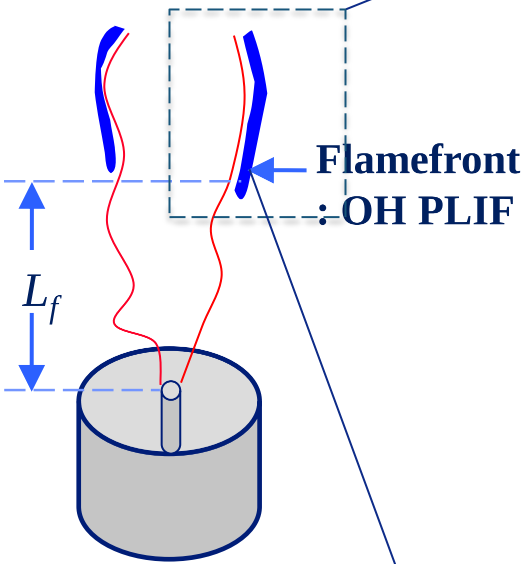
- Understand key phenomena and quantify rate-controlling process.
- Three world-leading experts (two at AFRL) and two Pecase awardees in the portfolio
- This area will be continuously supported with the following focuses:

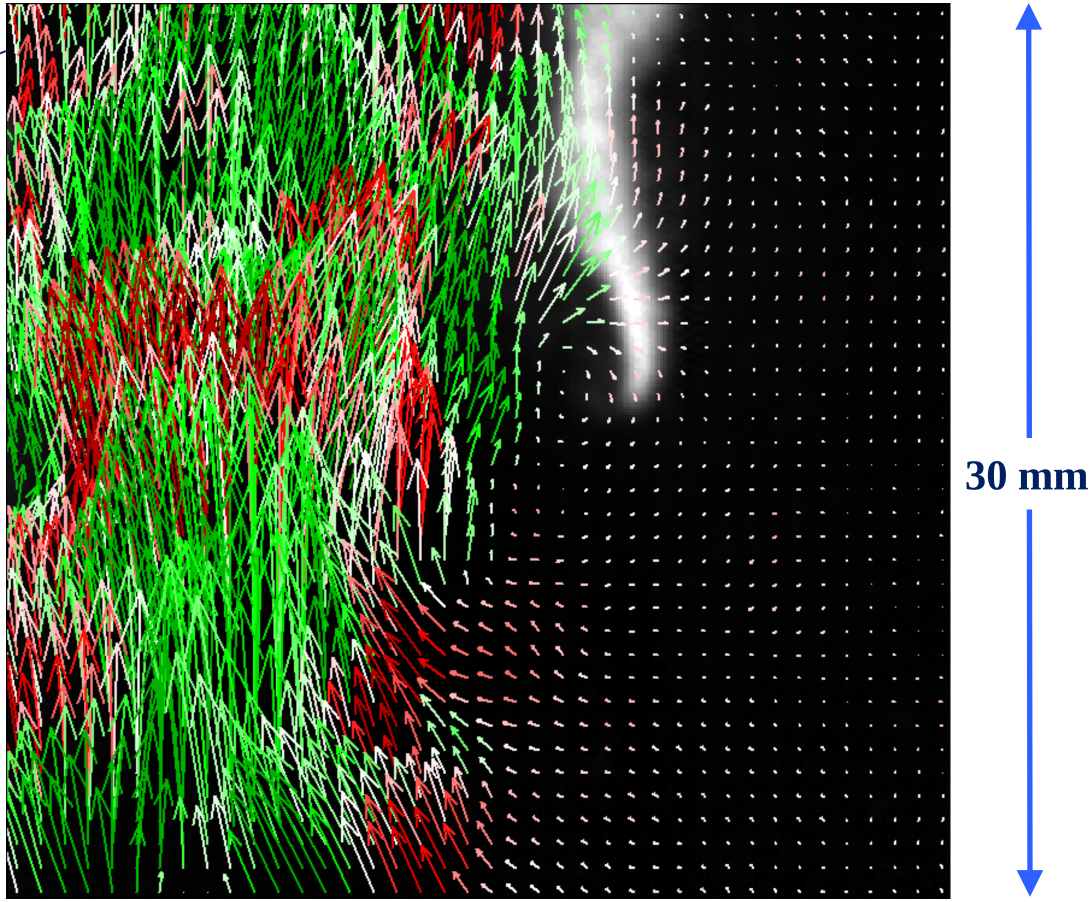
1. New signal generating processes and related basic spectroscopic approaches for key properties in chemically reacting flows;
2. Three-dimensional (volumetric or scanning two-dimensional) imaging approaches;
3. Techniques for multi-phase and spray combustion
4. Post processing capability to extract key physics from large-scale, multi-dimensional experimental data sets

Support Current Needs and Prepare for the Future

KHz Velocity-OH Imaging

KHz Imaging: (PI: Carter, AFRL/RZ)





$Re_j = 15k$: V_z magnitude shown with red and green OH shown in gray scale

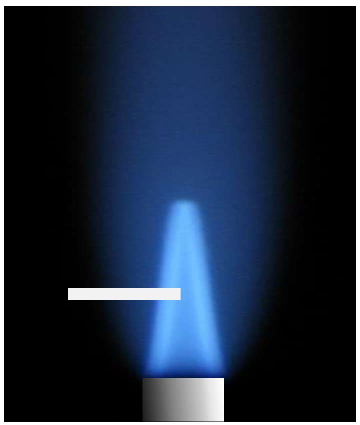
Simultaneously KHz Imaging of Velocity and OH Provide Multi-Dimensional, Time-Accurate Information on Flame and Flow

kHz, Interference-Free 2hν fs-Line-LIF Imaging of H Atom

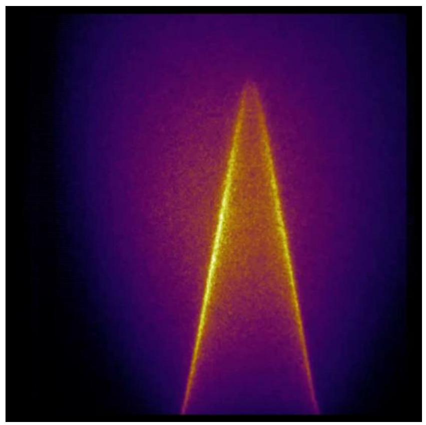
fs-Diagnostics: (PI: Gord, AFRL/RZ – working with Parra)

205-nm 2hν fs-LIF of H Atom

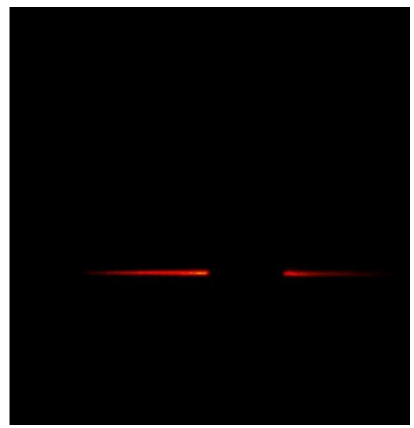
– Enjoys many of the same benefits as fs-CARS
– Reduces photolytic 1hν H atom production (H_2O, CH_3)
– kHz-rate 1D imaging

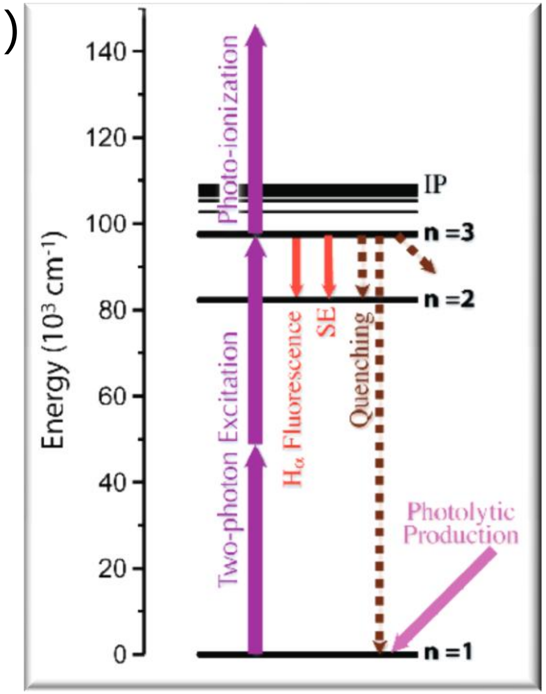


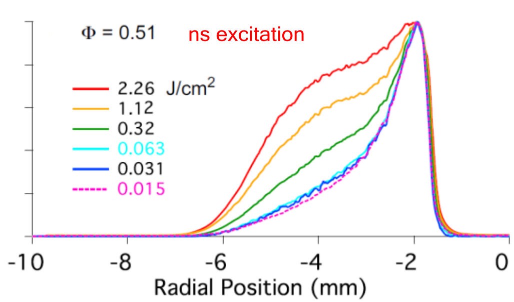
1-kHz Flame Luminosity

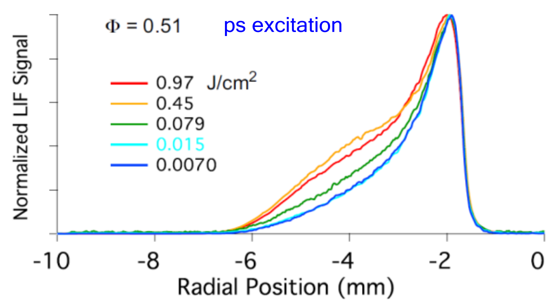


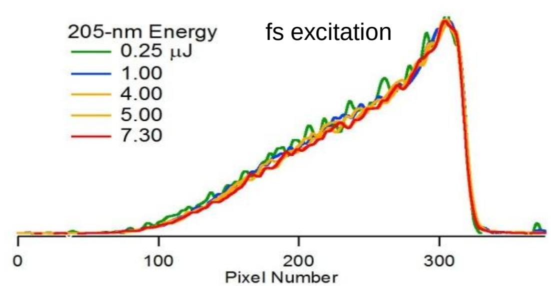
1-kHz fs-LIF







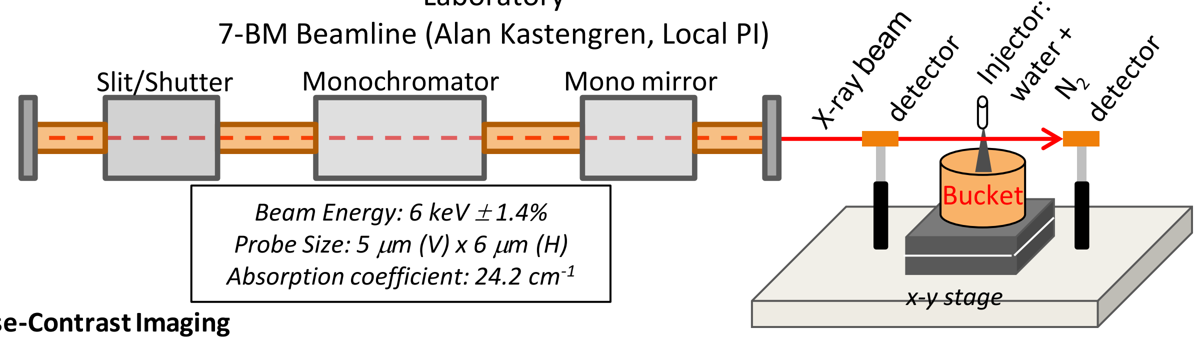




2hν with fs Laser Removes Probe-Beam Induced Interferences

X-Ray Multiphase Diagnostics: (PIs. Carter and Lin, AFRL/RZ)

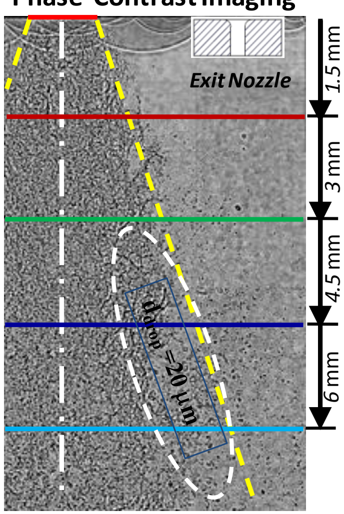
Collaborating with Advanced Photon Source, Argonne National Laboratory
7-BM Beamline (Alan Kastengren, Local PI)



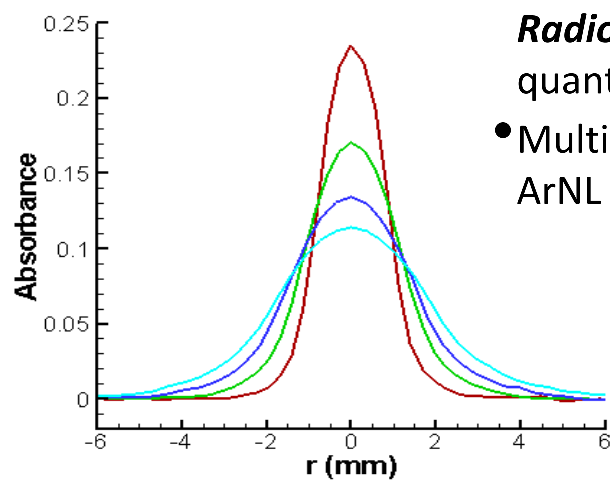
Probing of liquid fuel sprays:

- Crucial for high-speed multiphase combustion
- Extreme challenge:
- Combination of X-ray ***Phase Contrast Imaging (PCI)*** and ***Radiography*** provides quantitative diagnostic.
- Multi-year collaboration with ArNL

Phase-Contrast Imaging



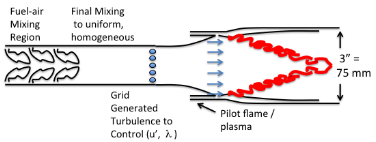
Left: *PCI of aerated spray showing high-res details*
Right*: radiography across spray showing quantitative distribution of liquid*



X-Ray Diagnostics is a Powerful Tool for Multi-Phase Flows; Particle Sizing Experiment Is On-Going for Super-Critical Injection Flows

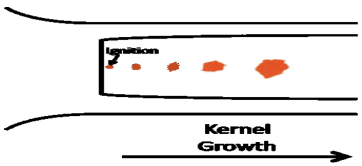
High-Re, High-M Turbulence Flame Experiments at AF Relevant Condition Ranges

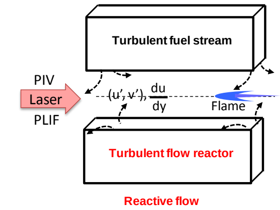
- Focus key combustion properties and characteristics such as:
    - ***Flame propagation,***
    - ***Flammability limit***
    - ***Combustion instability***
- Multi-phase conditions ***applicable*** to Air Force propulsion systems
- Made possible by diagnostics developed by this portfolio up to date



Key Requirements (Experimental Data Objectives):

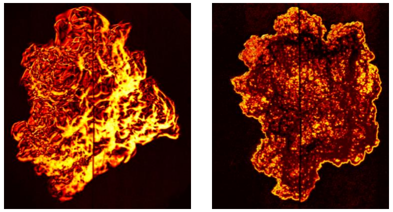
1. ***Understanding*** the above key combustion phenomena and characteristics;
2. ***Quantifying rate-controlling processes and scale****s* that govern those phenomena and characteristics;
3. Developing and validating as directly as possible ***basic model assumptions***
4. Controlling and quantifying turbulence properties are ***essential***.





Proposals are being considered and funded for:

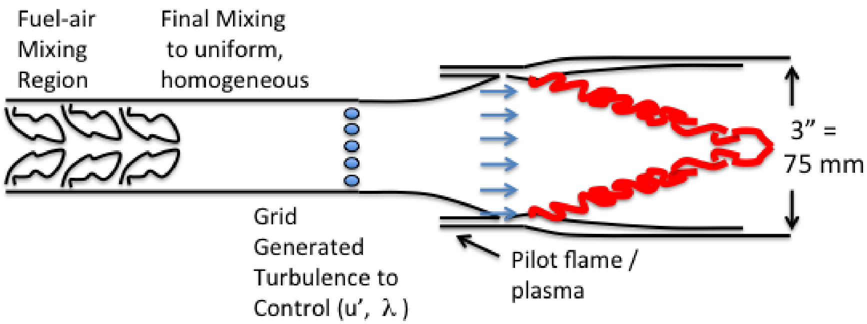
- Defining relevant conditions and Studying Critical Scales (1 funded in FY12)
- Relevant Experiments in different configurations (4 funded in FY12)

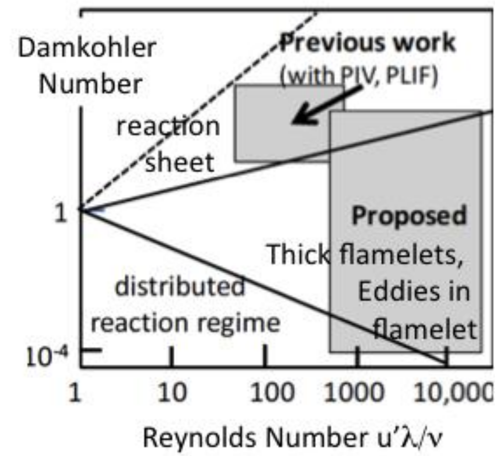


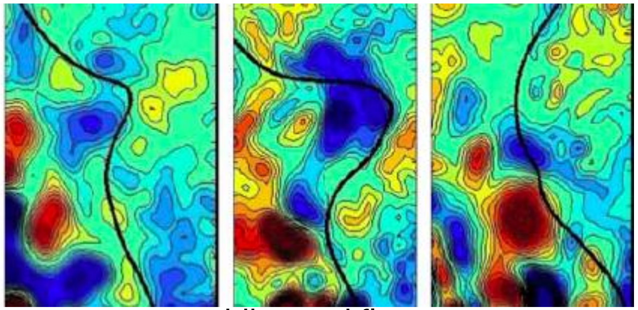
Understanding Starts from Observation and Data

U-Mich Experiment

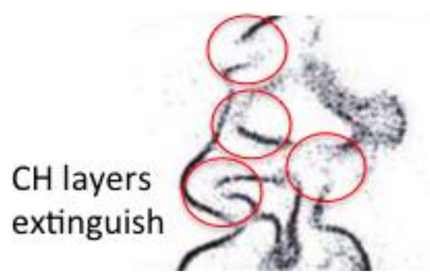
Premixed Turbulent Combustion in High Reynolds Number Regimes of Thick Flamelets and Distributed Reactions (PI: Driscoll – funded in FY12)







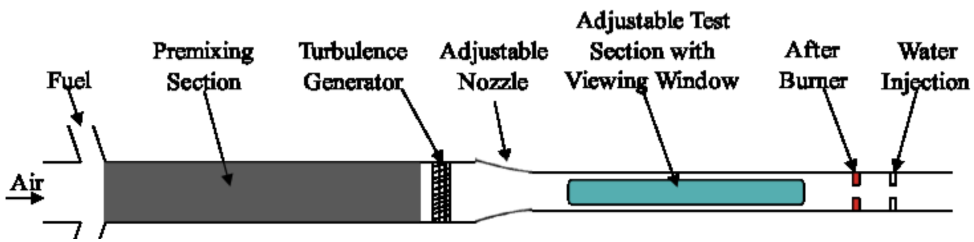
eddies and flame

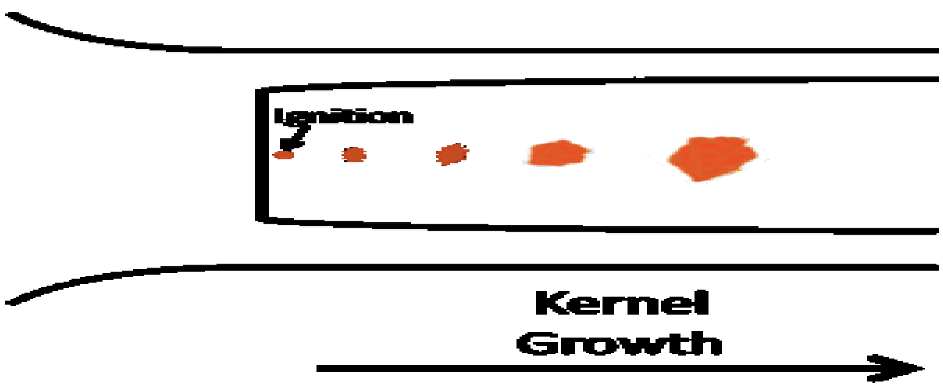


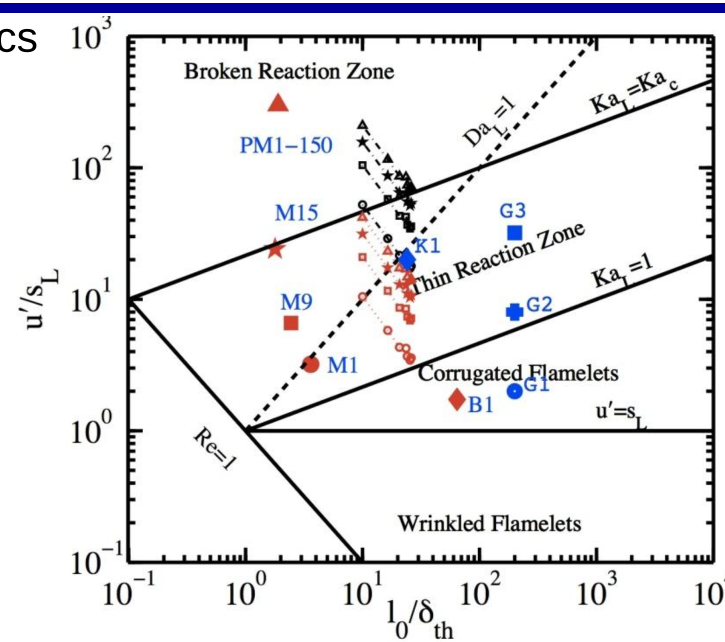
Turbulence-Flame Propagation from Pilot Regions: Studying Flame-Turbulence Interactions

G-Tech/VU Experiment

Premixed Flame Structure and Propagation Characteristics in Intense Turbulence and in Compressible Flow
(PI: Menon, Pitz and Lieuwen, funded in FY12)







- **Global (mean) flow and visualization**
  - **Pressure, temperature, flow rates, Schlieren, CH***
- **Turbulent flow field**
  - **2-component LDV: single & two-point (GT)**
    - Obtain mean, rms, spectra, integral scale
  - **10 KHz PIV (GT)**
  - **Hydroxyl Tagging Velocimetry (VU)**
  - **Compare results of LDV, PIV and HTV**
- **Flow-flame interactions and structures**
  OH-PLIF (GT/VU), CH2O-LIF (VU), flame edge (GT)
  UV-Raman (VU)

Un-Obstructed Flame Propagation in Highly Turbulent Compressible Flows

Combustion Modeling and Theory

1. ***Ab Initio*** Combustion Chemistry Modeling:
    - Reaction-set reduction approaches
    - Non-thermal-equilibrium reaction modeling
    - Supporting experiments, especially in the non-thermal-equilibrium area.
    - Closely working with chemistry colleagues

2. Physics Based Turbulence Combustion Modeling
    - Based on key understanding from experimental data (beyond simple parameter fitting)
    - More ab Initio when possible

3. Numerical Experiments, i.e. use simulations as an experimental tools to:
    - Qualitatively explore key combustion phenomena
    - Obtain fundamental understanding
    - Identify rate-controlling processes and scales
    - Develop more experiment-independent, quantitative numerical experimental approaches

4. Combined experimental-numerical approaches:
    - Numerical simulations ***coupled, fused or constrained*** with experimental data
    - Providing information otherwise not available from experimental measurements
    - Pull solution process in the correct direction (similar to what used in the meteorology area)

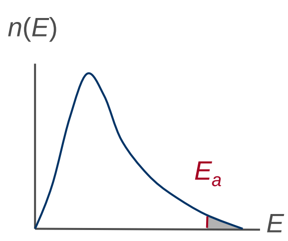
5. Numerical capability to analyze large-scale data sets from numerical simulations to ***extract key physics***

Combustion Chemistry Modeling Beyond Arrhenius Model

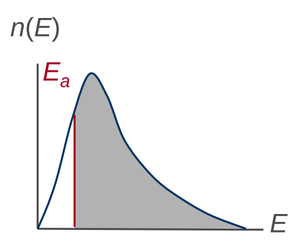
Current Base-Line Model for a Single Reaction step:

- Arrhenius Model:
  - works for high activation energy reactions
- breaks down:
  - with many large molecules (e.g., low energy barrier reaction)
  - at high-temperature thermally non-equilibrium conditions (e.g. high-speed flow or cross strong shock)

$k(T) = AT^{n}e^{-Ea/RT}$

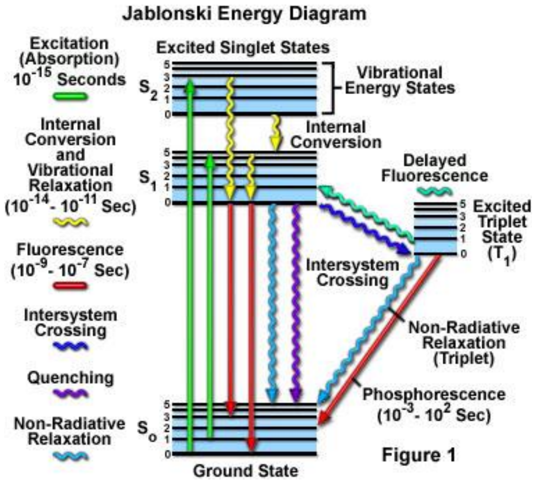


$k(T) = ?$



First-Principle Methods

Theories for Thermally Non-equilibrium Condition

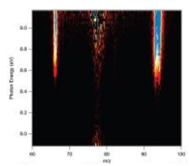


- Determine relaxation time scale using master equation modeling of collision energy transfer
- Direct solution of Boltzmann equation
- Experimental observation, e.g., ps/fs CARS imaging of relaxation process (e.g. during a shock)
- **Perspective**: critical to supersonic combustion modeling

New Exploratory Area Considered by This Portfolio

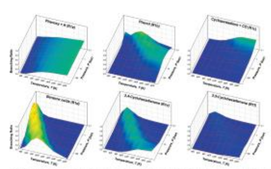
Combustion Chemistry Modeling: *Ab Initio* Approaches for Rate-Constants and Set-Reduction

First-Principle Methods



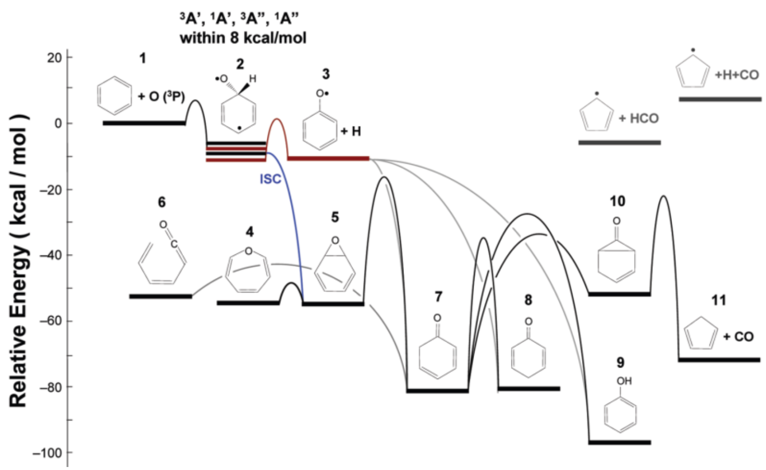
Ab Initio Rate Const. Computations

- potential energy surface by ab initio electronic structure calculation
- $k(T,P)$ determined using master equation modeling
- usually require comparison with data, e.g., synchrotron photo-ionization mass-spectrometry
- **Perspective**: accurate yet impractical with the large number of reactions to be considered



rate const. calculated with RRKM/master equation modeling

Currently funded by DOE and AFOSR



Ab Initio Reaction Set Reduction

- use Gibbs potential energy surface to weed out noncritical pathways
- interrogate local energy barriers along probable paths
- determine the reaction time scale and critical rate constants by first-principle methods as needed
- isolated shock-tube experiments to pinpoint the rate limiting step
- **Perspective**: minimize critical information needed for turbulent reacting flow simulations

New Exploratory Area Considered by This Portfolio

Innovative Combustion Approach

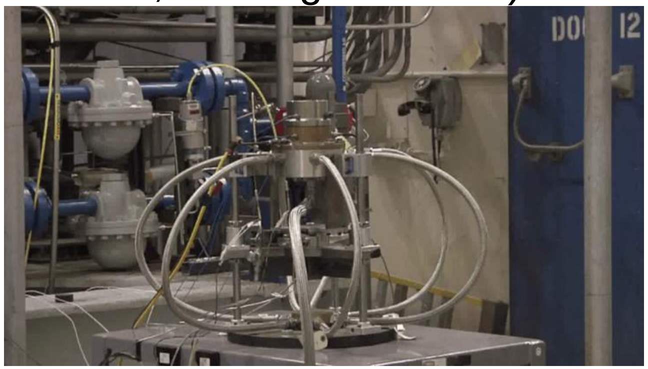
Looking for innovative, game-changing research activities:

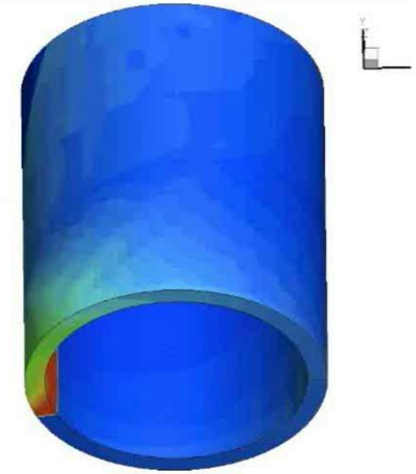
- •explored new concept of converting chemical to mechanical energy
- •new combustion regimes
- •new fuels:

1. Rotational or Continuous Detonation (intense/concentrated combustion);
2. Flameless combustion (distributed combustion process);
3. Plasma and catalytic assisted combustion process (creating a new rate-controlling process);
4. Direct conversion from chemical energy to mechanical energy, including bio-inspired approaches, (e.g. bio-inspired processes);
5. Alternative fuel of superior physical and combustion/energy-conversion properties with favorable source-characteristics.

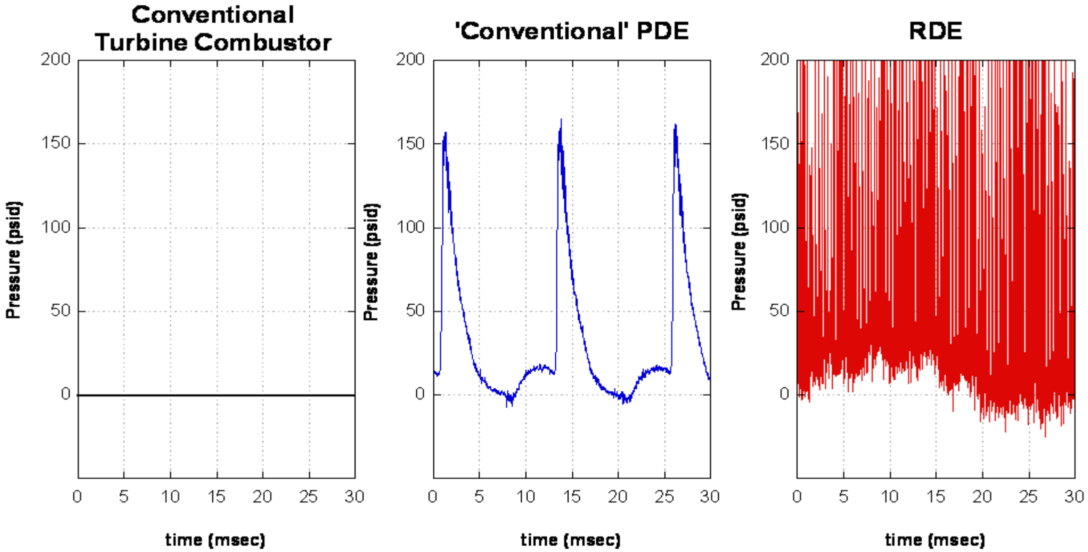
Rotational/Continuous Detonation

Rotational Detonation: (PI: Schauer, AFRL/RZ, working with NRL)





*CFD Courtesy of NRL



- **Only Single Initiation needed (Circumvent Initiation/DDT difficulty/loss in PDE)**
- **10-100x cycle rate increase**
- **Near Steady Exit Flow**

Rotational Approach Allows Continuous Detonation - A Game Changer

Summary and Looking Forward

Advance of diagnostics (continuous investments)***:***

- •Support current experiment needs (e.g. compressible, high-M-Re turbulence combustion experiments);
- •Open new research capability.

Turbulence Combustion Experimental Efforts (new focus)***:***

- •Understand turbulence flame properties, quantify rate-controlling in regains of AF interest;
- •Develop/validate basic model assumptions;
- •High-quality data sets with well defined conditions for long-term community use:
  - •Gas-phase combustion data, 2~3 years, then, move to multiphase, supercritical conditions;
  - •This experimental focus on turbulence combustion -- expected to complete in about 4-5 years.

Combustion Modeling and Theory (new focus with existing elements)***:***

- •Ab Initio and more computationally efficient combustion chemistry models;
- •Physics base turbulence combustion model assumptions/ models;
  - •Based on key understanding from experimental data (beyond simple parameter fitting);
  - •More ab. Initio when possible;
- •Numerical experiments and combined numerical-experiment (physical) approaches– a game changer;
- •Numerical capability to analyze large-scale data sets (simulation or experiment) to extract key physics.

Innovative Energy Conversion/Combustion Processes (new focus with existing elements)***:***

- •Explored new concept of converting chemical to mechanical energy (e.g. bio-inspired);
- •New combustion regimes;
- •New fuels.

Recent Transitions

Advanced Diagnostics (RZT : for F-22 and T-38 Engines):

- High-speed (kHz) digital imaging and planar laser visualization of fuel spray spatial distribution and morphology
- Phase Doppler particle analysis (PDPA) for fuel spray droplet-size and velocity distributions
- Temperature and water-concentration measurements along multiple lines of sight.

JetSurF Combustion Kinetics Set (UCS: for RZ and PW):

- Simulation tools for engine exhaust predictions

Closing Statements

Keep Exploring:
Go Where No-One Has Gone Before!