



Integrity ★ Service ★ Excellence

Energy Conversion and Combustion Sciences

08 MAR 2012

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Report Documentation Page				Form Approved OMB No. 0704-0188	
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1. REPORT DATE 08 MAR 2012		2. REPORT TYPE		3. DATES COVERED 00-00-2012 to 00-00-2012	
4. TITLE AND SUBTITLE Energy Conversion And Combustion Sciences				5a. CONTRACT NUMBER	
				5b. GRANT NUMBER	
				5c. PROGRAM ELEMENT NUMBER	
6. AUTHOR(S)				5d. PROJECT NUMBER	
				5e. TASK NUMBER	
				5f. WORK UNIT NUMBER	
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) Air Force Research Laboratory, Wright-Patterson AFB, OH, 45433				8. PERFORMING ORGANIZATION REPORT NUMBER	
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)				10. SPONSOR/MONITOR'S ACRONYM(S)	
				11. SPONSOR/MONITOR'S REPORT NUMBER(S)	
12. DISTRIBUTION/AVAILABILITY STATEMENT Approved for public release; distribution unlimited					
13. SUPPLEMENTARY NOTES					
14. ABSTRACT					
15. SUBJECT TERMS					
16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT Same as Report (SAR)	18. NUMBER OF PAGES 26	19a. NAME OF RESPONSIBLE PERSON
a. REPORT unclassified	b. ABSTRACT unclassified	c. THIS PAGE unclassified			



2012 AFOSR SPRING REVIEW



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:

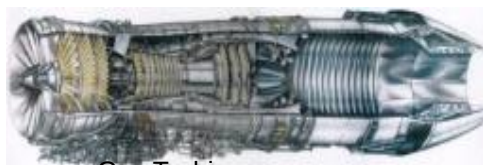
- One of **most important** determining factors of operability and performance;
- One of **least understood** areas in basic combustion research, with large uncertainties;
- Confluence of a “grand-old” fundamental science problem, immediate needs and long-term interests;
- Recent advances in diagnostics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



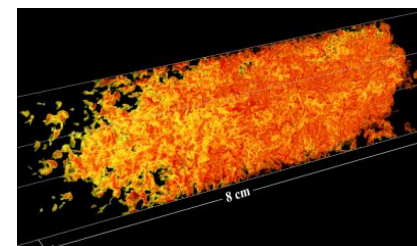
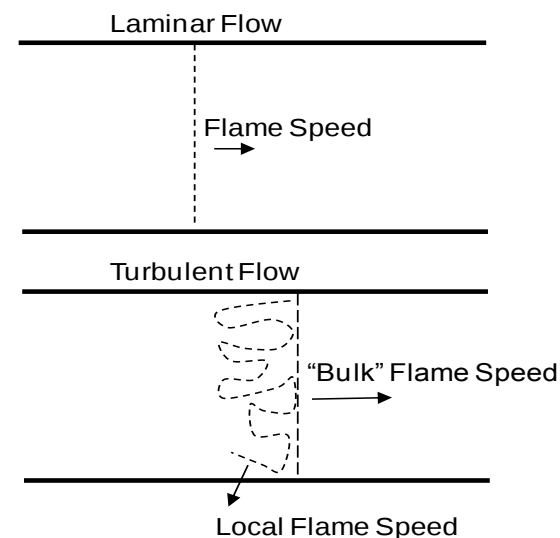
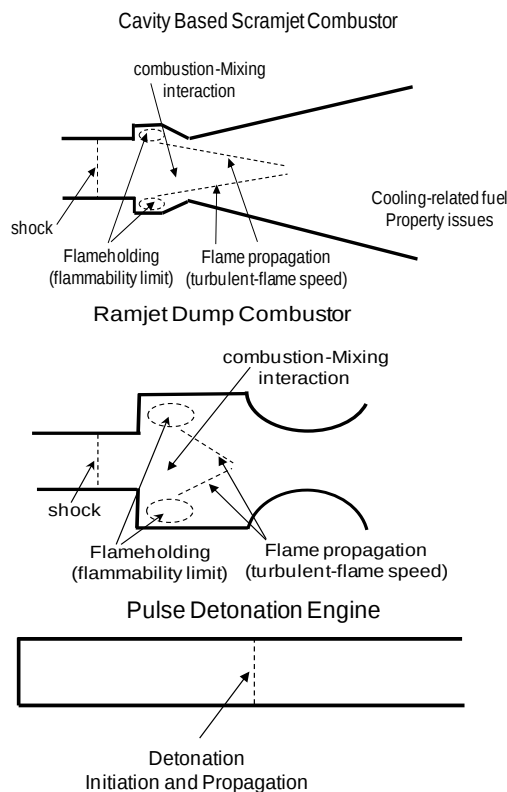
Rockets



Hypersonics

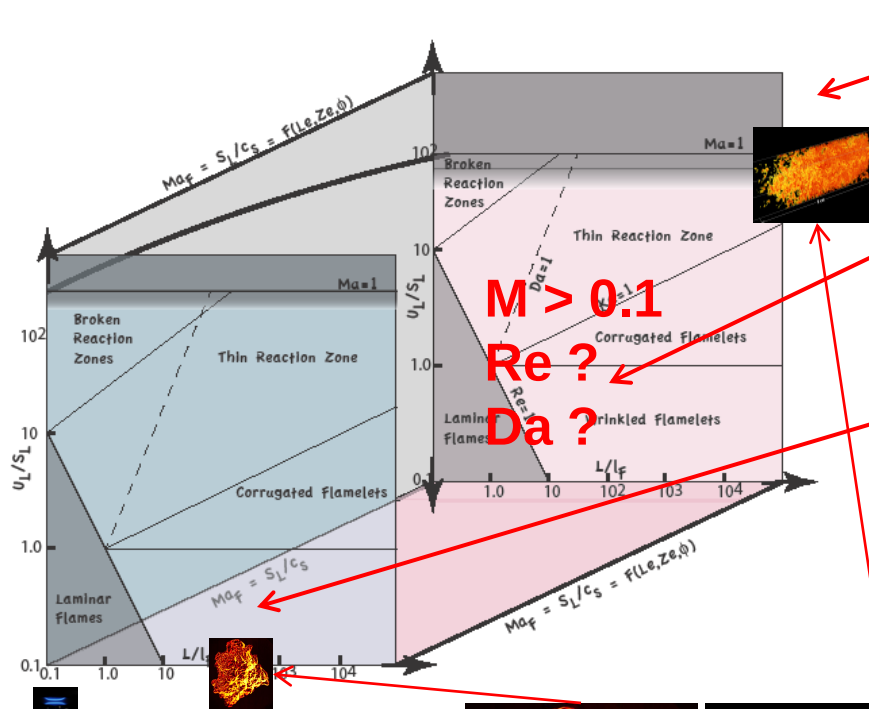


Gas Turbines

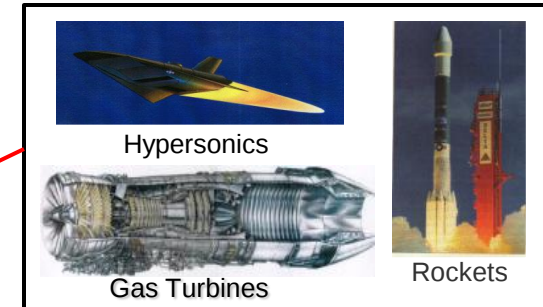




Turbulence Combustion: Fundamental Structures, Critical Scales and Relevant Conditions



RDE/PDE

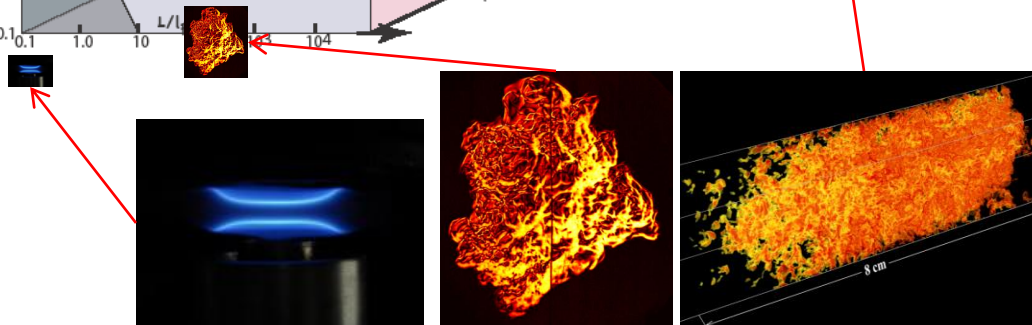


Auto Engines

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

Key Questions:

- Flame Structure?
- Regime Boundaries?
- Critical Scales?
- Relevant Conditions?
- Rate-Controlling Processes?



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

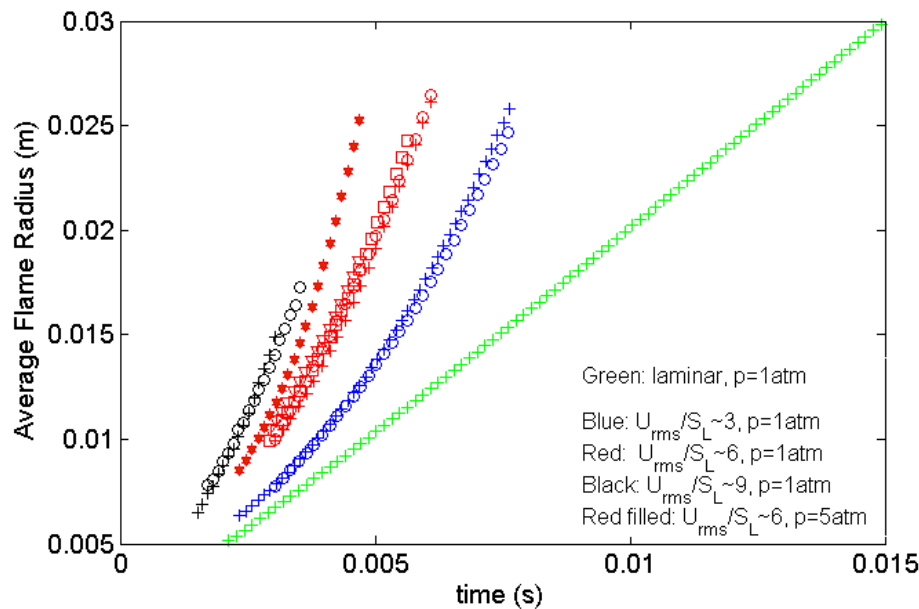
- (1) Little Data Available at Compressible, High-Re Conditions;
- (2) Needs for Better Definition of Re-Conditions in Regions of Interests



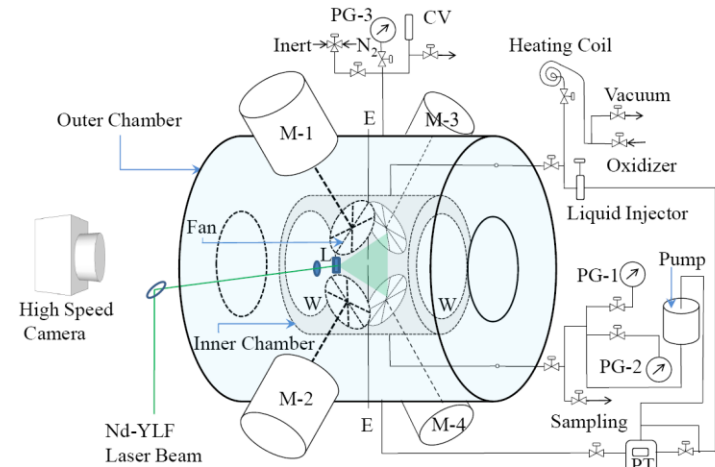
Low-Re Bounding Experiment (Physical)



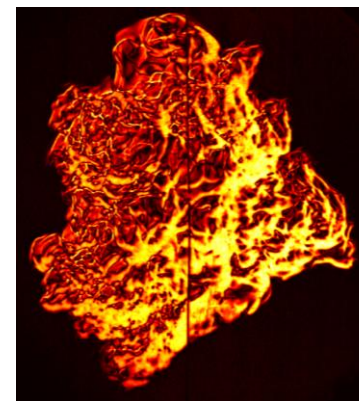
Flame Speed and Self-similar Propagation of Turbulent Premixed Flames: (PI: Law, Princeton)



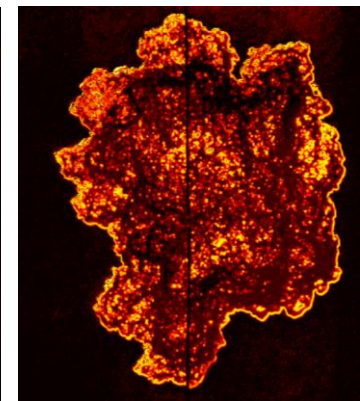
Turbulence Already Affects Flame Structure and Speed at Relatively Low Re Conditions



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



Pressure = 1atm



Pressure = 5atm

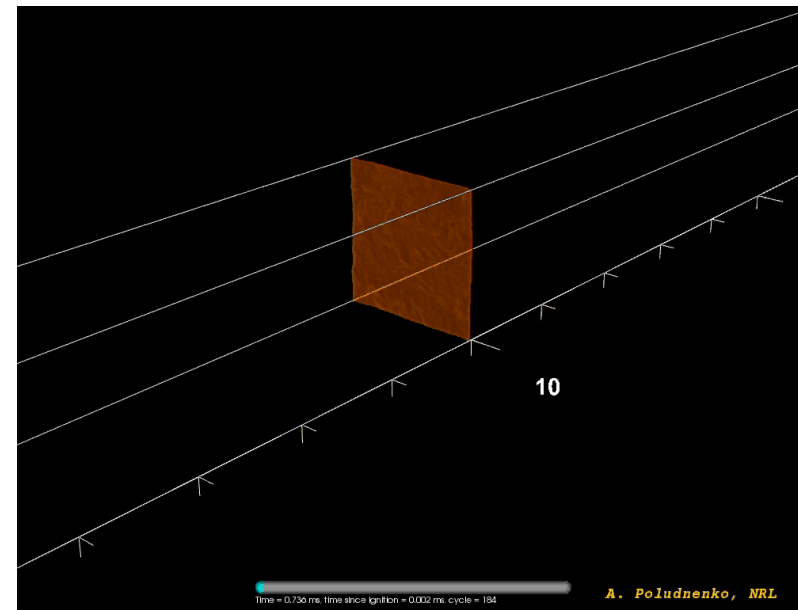
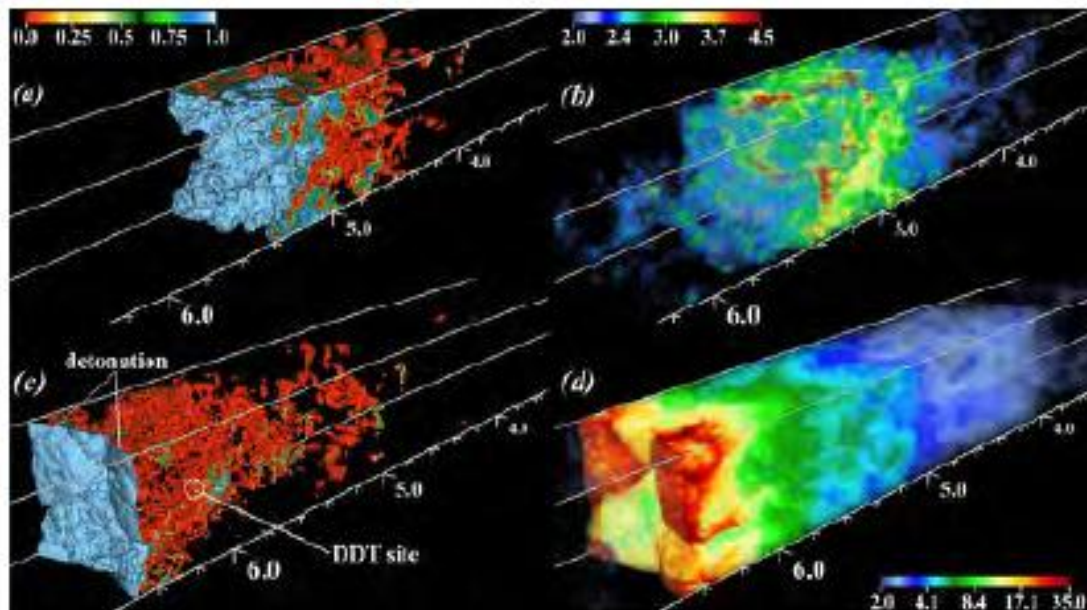
Schlieren images of turbulent premixed CH_4/air flames ($\phi=0.9$, $Le=1$) at same u_{rms}



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)

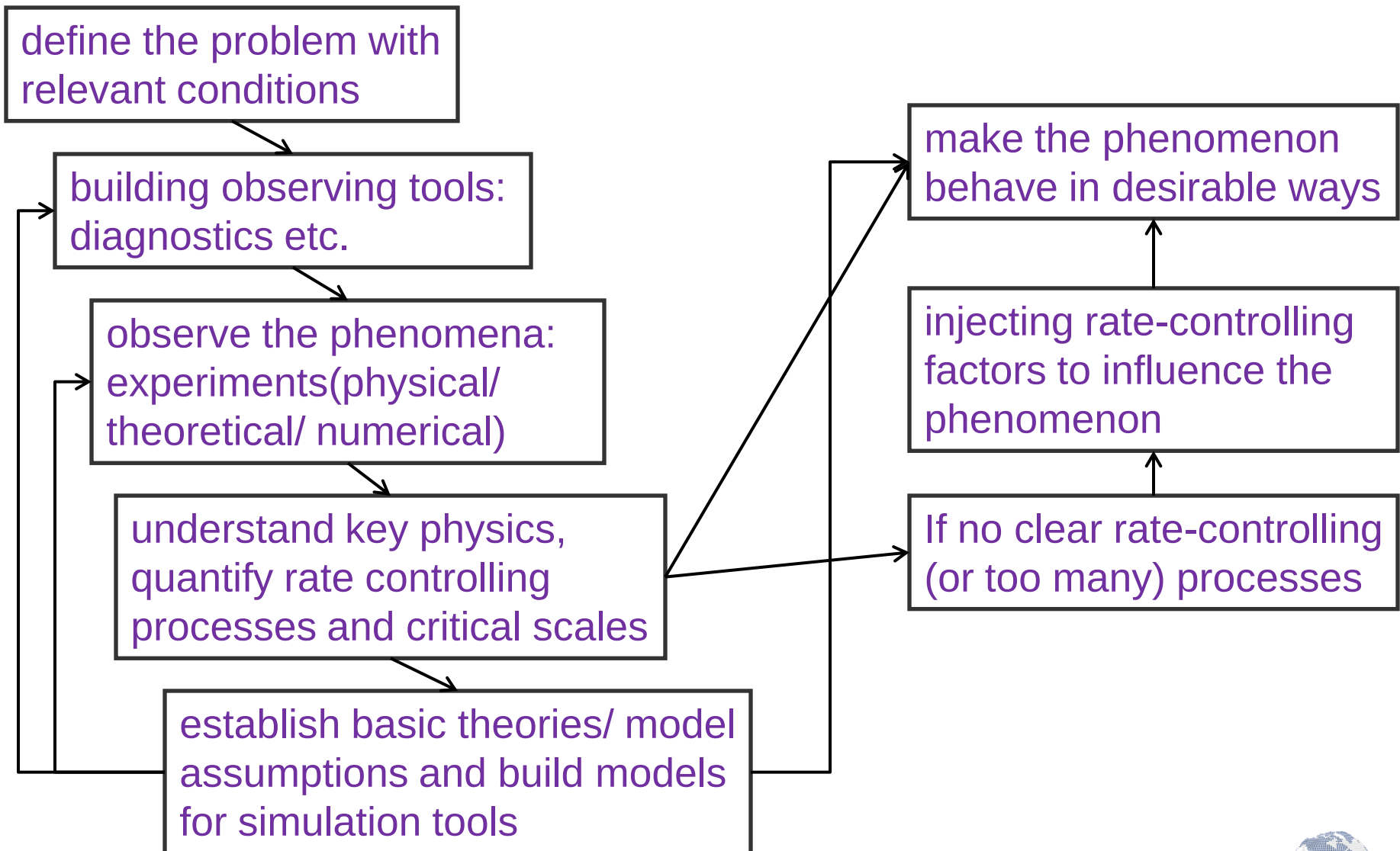
4. Numerical and Mathematical Issues

- 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:

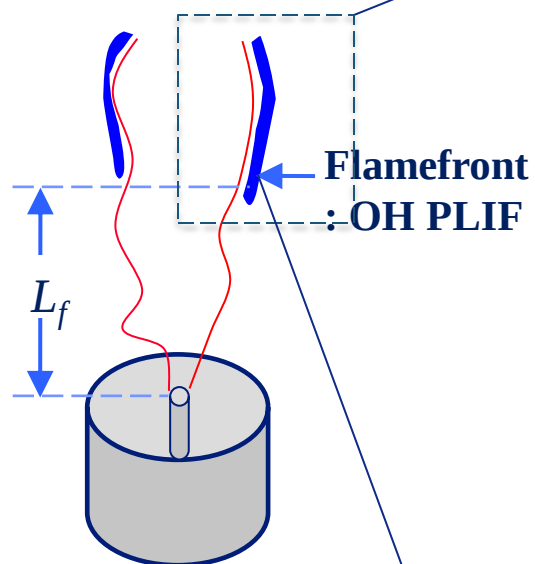
1. New signal generating processes and related basic spectroscopic approaches for key properties in chemically reacting flows;
2. Three-dimensional (volumetric or scanning two-dimensional) imaging approaches;
3. Techniques for multi-phase and spray combustion
4. Post processing capability to extract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

Support Current Needs and Prepare for the Future

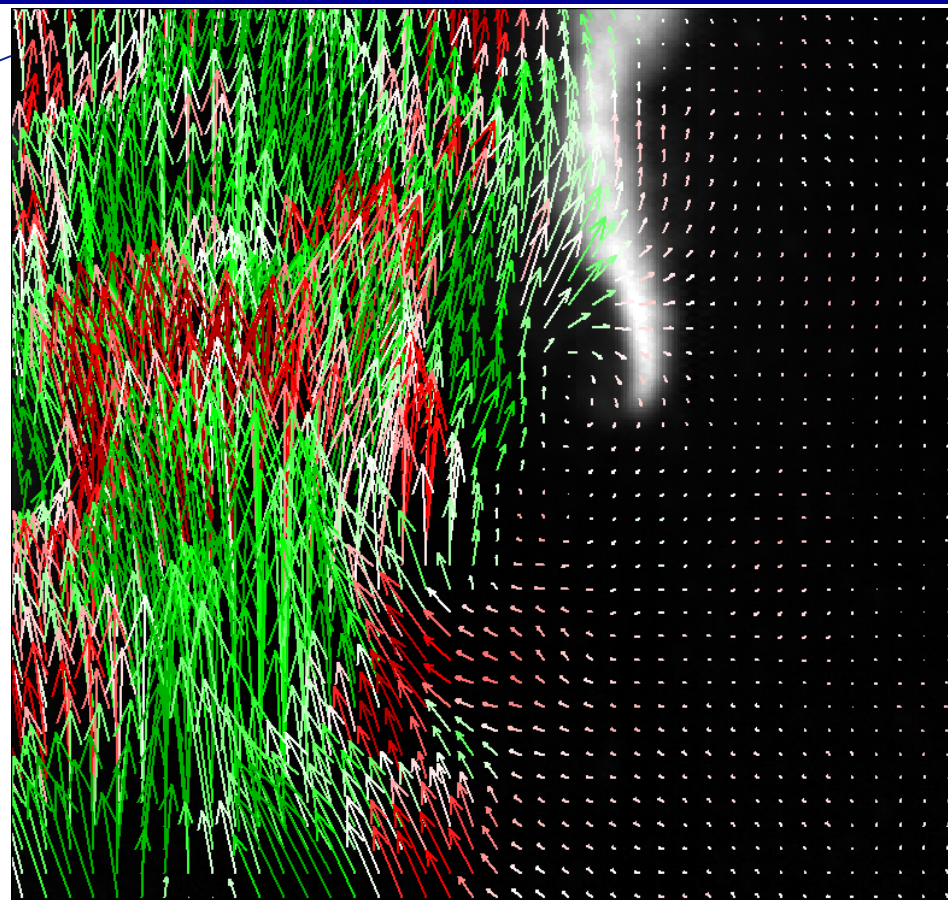


KHz Velocity-OH Imaging

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



Fuel Jet: Propane+Argon;



30 mm

$Re_j = 15k$: 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 2h ν fs-Line-LIF Imaging of H Atom

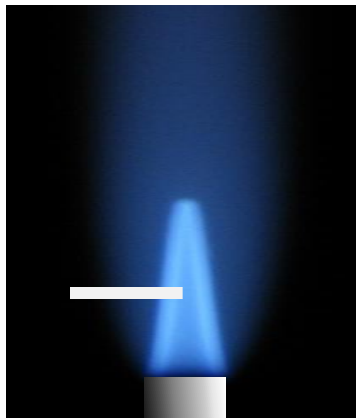


fs-Diagnostics: (PI: Gord, AFRL/RZ – working with Parra)

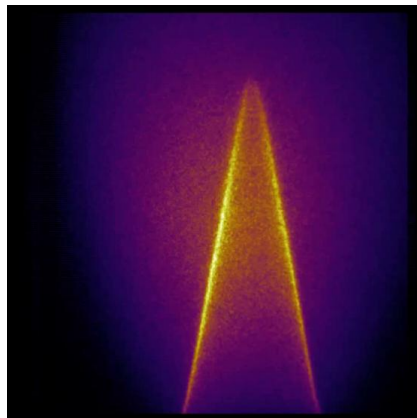
205-nm 2h ν fs-LIF of H Atom

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

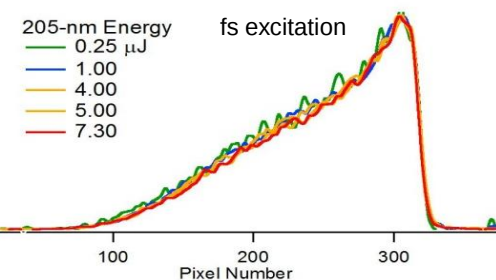
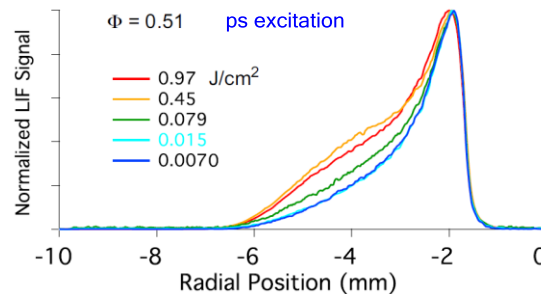
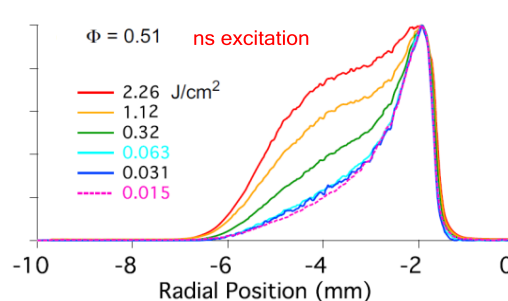
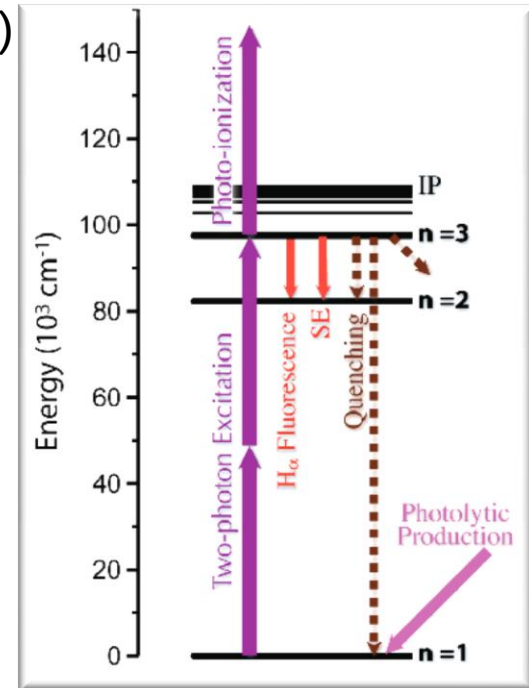
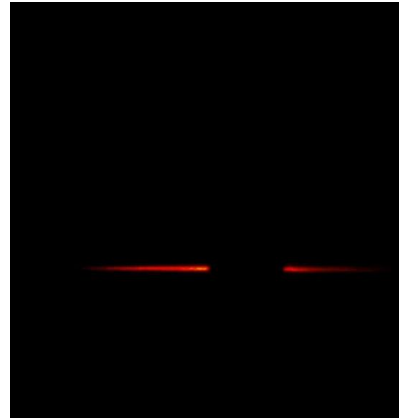
1-kHz Flame Luminosity



1-kHz fs-LIF



1-kHz fs-LIF



2h ν with fs Laser Removes Probe-Beam Induced Interferences



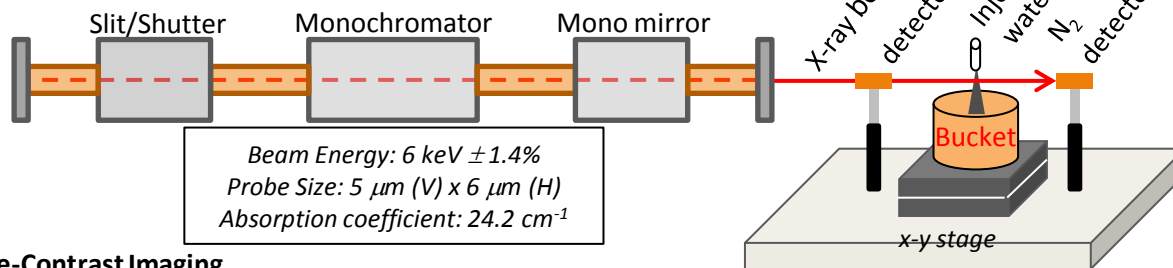
X-Ray Multiphase Diagnostics



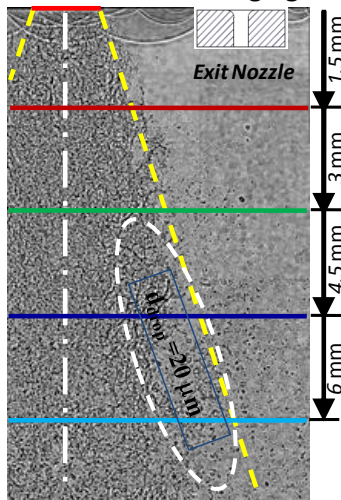
X-Ray Multiphase Diagnostics: (Pls. Carter and Lin, AFRL/RZ)

Collaborating with Advanced Photon Source, Argonne National Laboratory

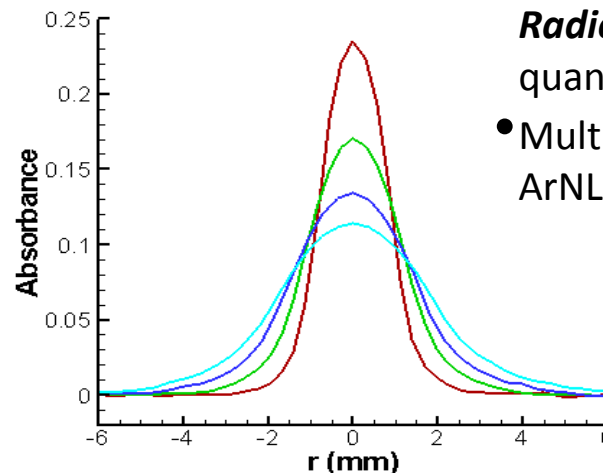
7-BM Beamline (Alan Kastengren, Local PI)



Phase-Contrast Imaging



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



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

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



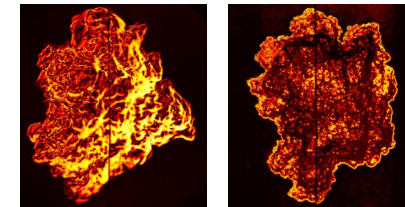
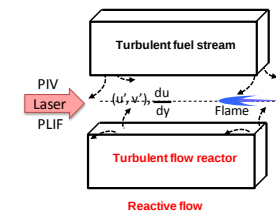
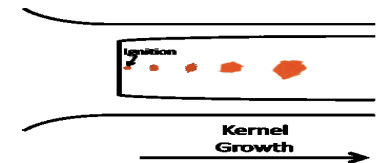
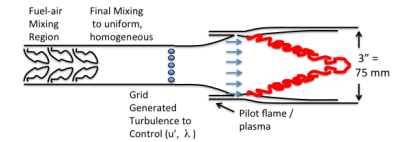
- Focus key combustion properties and characteristics such as:
 - **Flame propagation**,
 - **Flammability limit**
 - **Combustion instability**
- Multi-phase conditions **applicable** to Air Force propulsion systems
- Made possible by diagnostics developed by this portfolio up to date

Key Requirements (Experimental Data Objectives):

1. **Understanding** the above key combustion phenomena and characteristics;
2. **Quantifying rate-controlling processes and scales** 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)



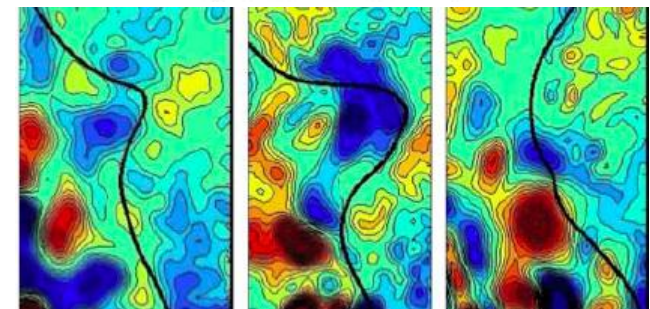
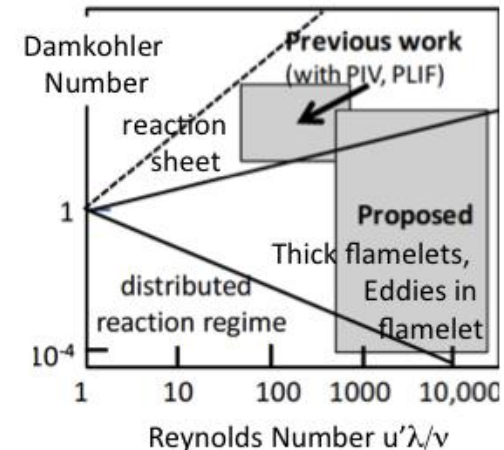
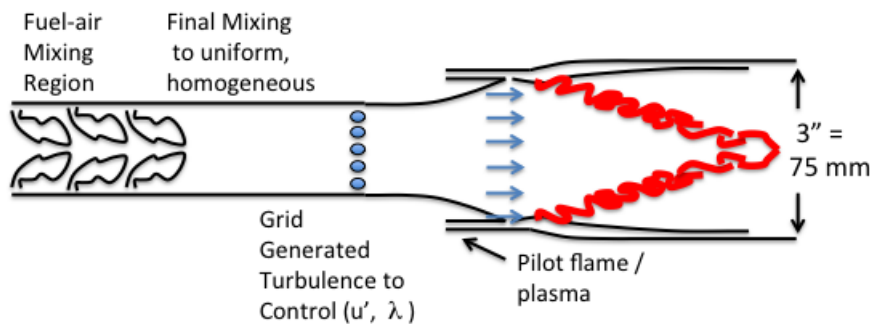
Understanding Starts from Observation and Data



U-Mich Experiment

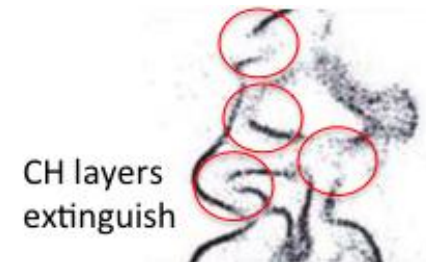


Premixed Turbulent Combustion in High Reynolds Number Regimes of Thick Flamelets and Distributed Reactions (PI: Driscoll – funded in FY12)



eddies and flame

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



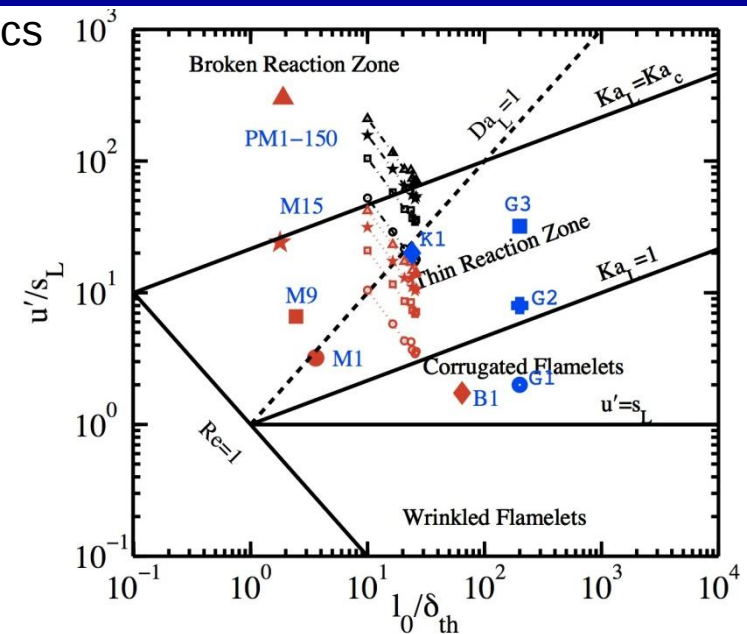
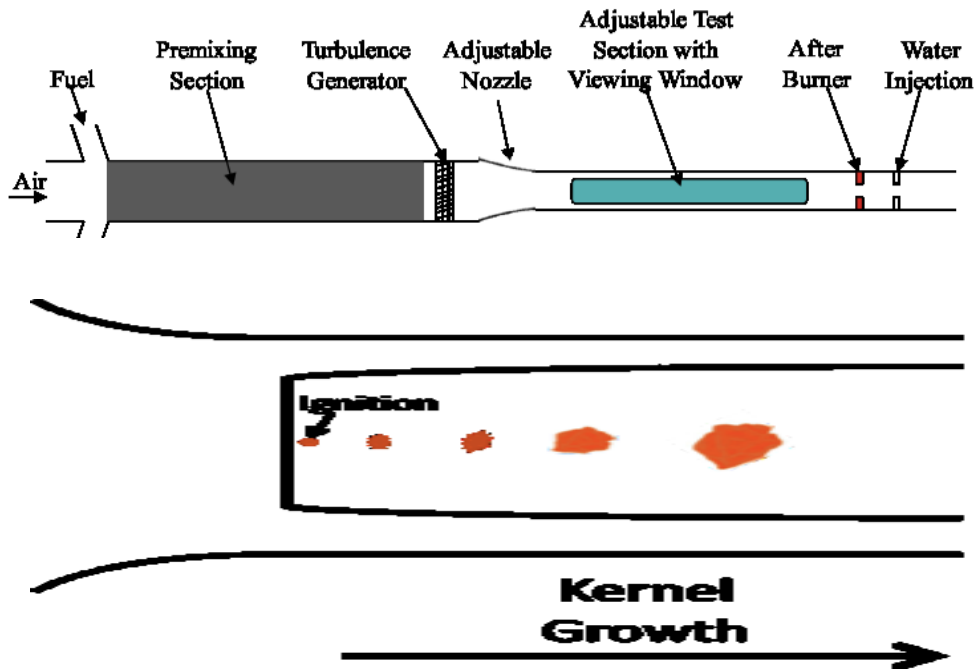
CH layers
extinguish



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

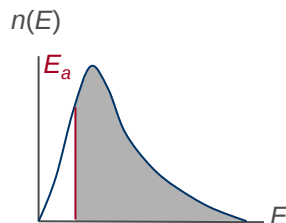
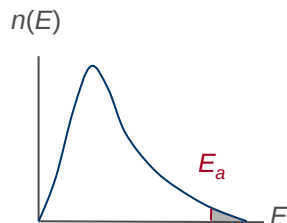


Current Base-Line Model for a Single Reaction step:

- 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)

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

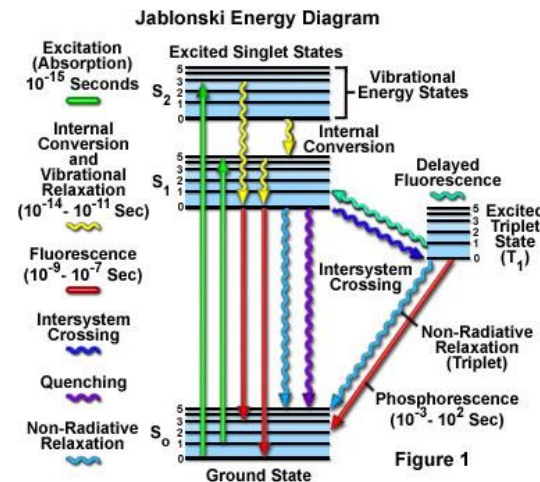
$$k(T) = ?$$



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

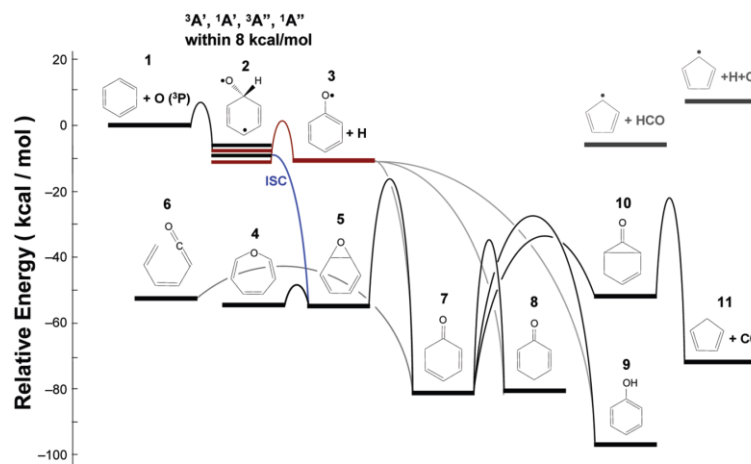
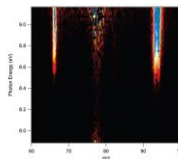
New Exploratory Area Considered by This Portfolio



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

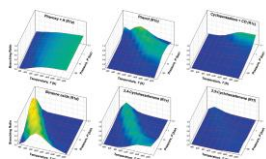


First-Principle Methods



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

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

Currently funded by DOE and AFOSR

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:

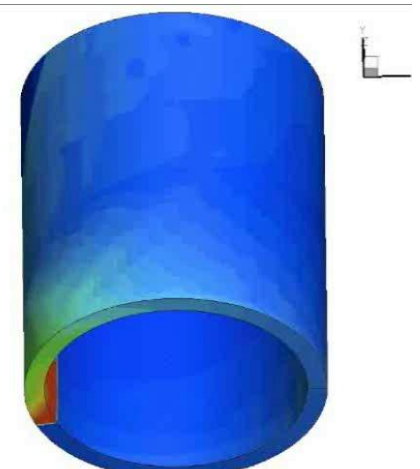
1. Rotational or Continuous Detonation (intense/concentrated combustion);
2. Flameless combustion (distributed combustion process);
3. Plasma and catalytic assisted combustion process (creating a new rate-controlling process);
4. Direct conversion from chemical energy to mechanical energy, including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



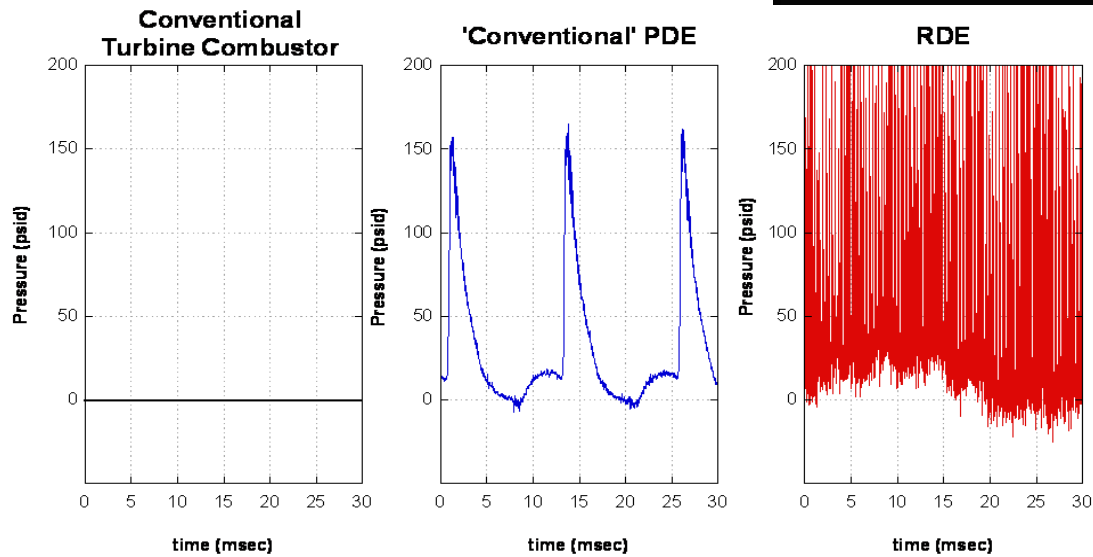
Rotational/Continuous Detonation



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!