A Joint Experimental/Computational Study of Non-idealities in Practical Rotating Detonation Engines

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Summary

- **Title:**
  - A Joint Experimental/Computational Study of Non-idealities in Practical RDEs
- **Funding agency:**
  - University Turbine Systems Research/NETL
  - Funding Opportunity Number: DE-FOA-0001248
  - Topic Area 2: Pressure Gain Combustion R&D
  - Project manager: David Lyons
- **Personnel:**
  - PI: Mirko Gamba, University of Michigan
  - Co-I: Venkat Raman, University of Michigan
  - Students currently involved:
    - Fabian Chacon
    - Yasin Abul-Huda
    - Chadwick Harvey
    - Romain Fievet
  - Key external collaborators:
    - Dr. John Hoke, Innovative Scientific Solution, Inc. (ISSI)
    - Drs. Adam Holley and Peter Cocks, United Technology Research Center (UTRC)
    - Dr. K. Kailasnath, Navy Research Labs (NRL)

Outline

- Introduction to the problem and general approach
- Experimental activities
- Computational activities

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Overarching objectives

- **Objective 1:**
  Develop canonical and operational RDE configurations, as well as imaging-based laser diagnostics for understanding fuel stratification, leakage, parasitic combustion and detonation structure under non-ideal conditions in RDEs.

- **Objective 2:**
  Develop a comprehensive picture of the fundamental physics governing non-idealities and how they impact RDE performance and operability from both experiments and simulations.

- **Objective 3:**
  Develop detailed computational tools (DNS & LES) for studying detonation wave propagation processes in RDEs to aid design.

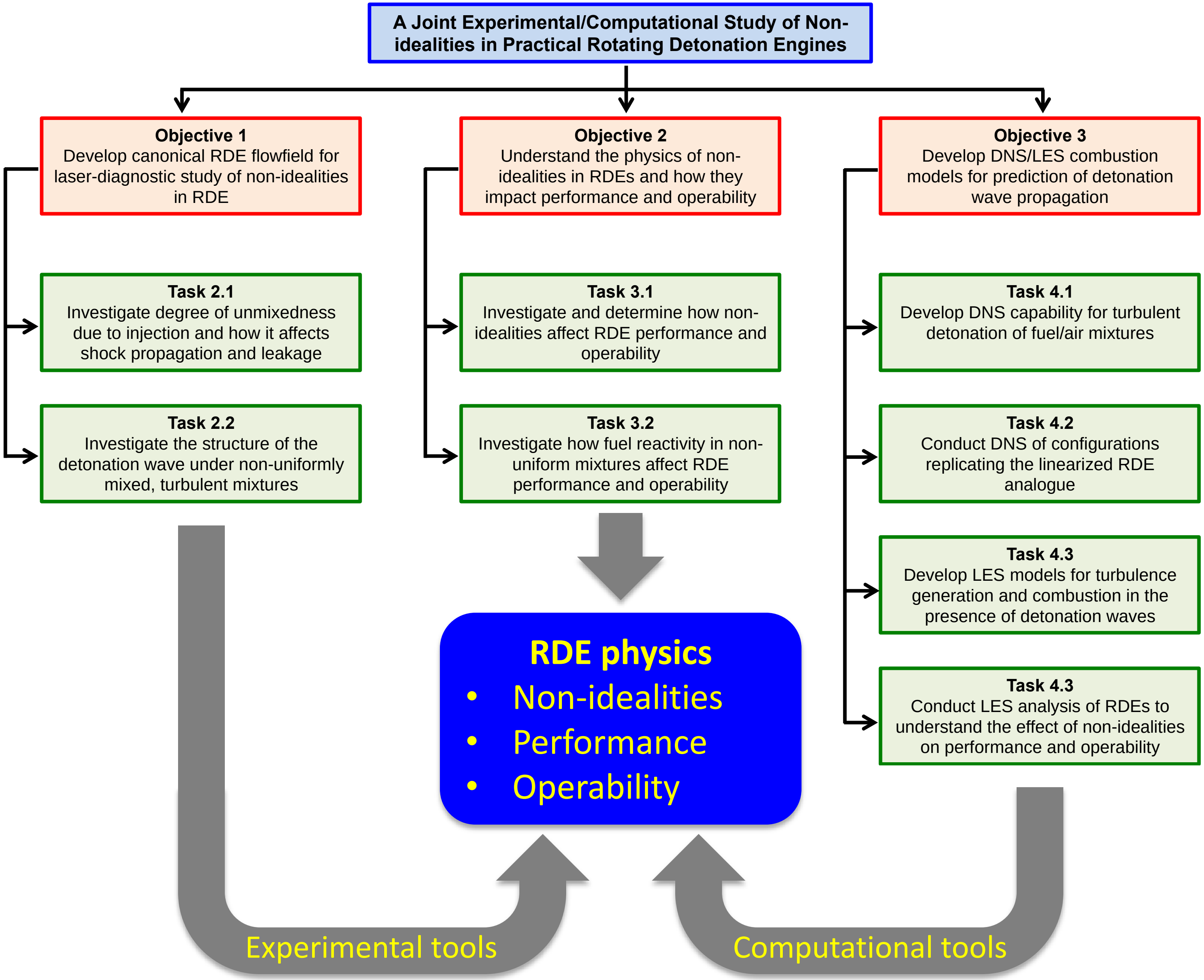
Expected outcomes

- **Outcome 1:**
  Identify the sources and properties of non-idealities in RDEs, their contribution to loss in pressure gain, and potential design limitations

- **Outcome 2:**
  Detailed experimental tools and measurements (databases) about fundamental aspects of RDEs will become available to the RDE design community.
  - e.g., transfer of techniques and data to DOE/NETL, UTRC, ISSI, NRL

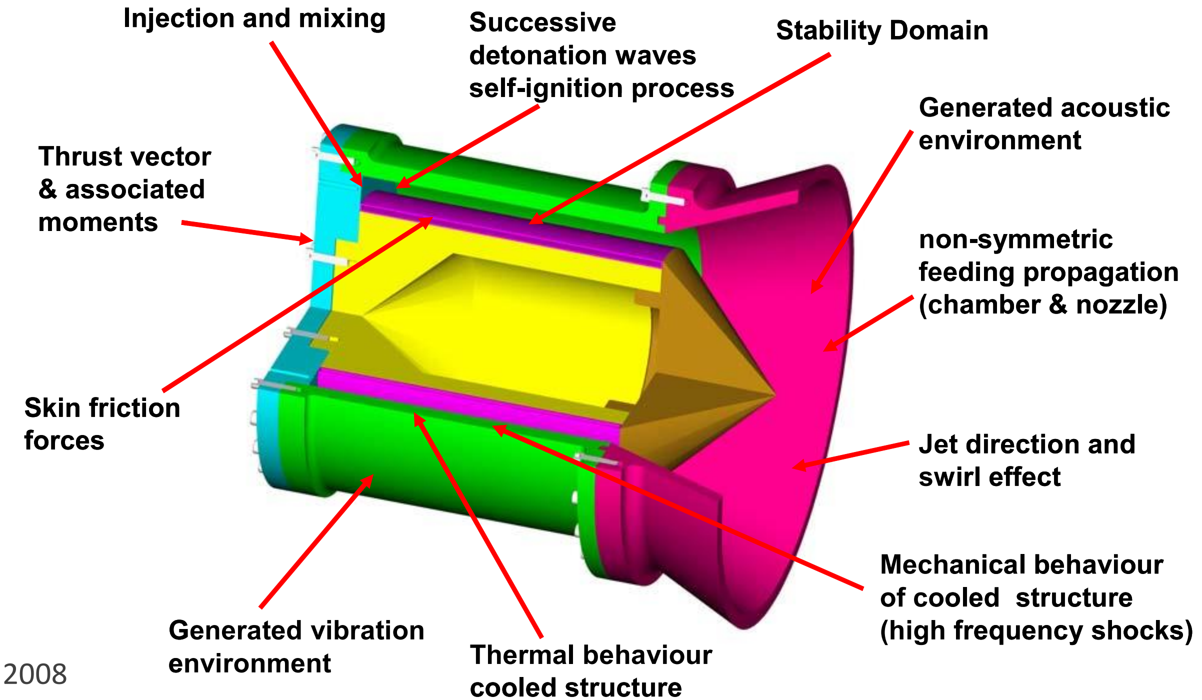
- **Outcome 3:**
  Detailed computational tools (DNS/LES) as well as combustion models with detailed chemistry for pressure gain combustion will be made available to the RDE design community.
  - e.g., openFoam development of RDE modeling
  - e.g., transfer of detonation computational models to DOE/NETL, UTRC, ISSI, NRL

Objectives and tasks



(Some) Practical challenges

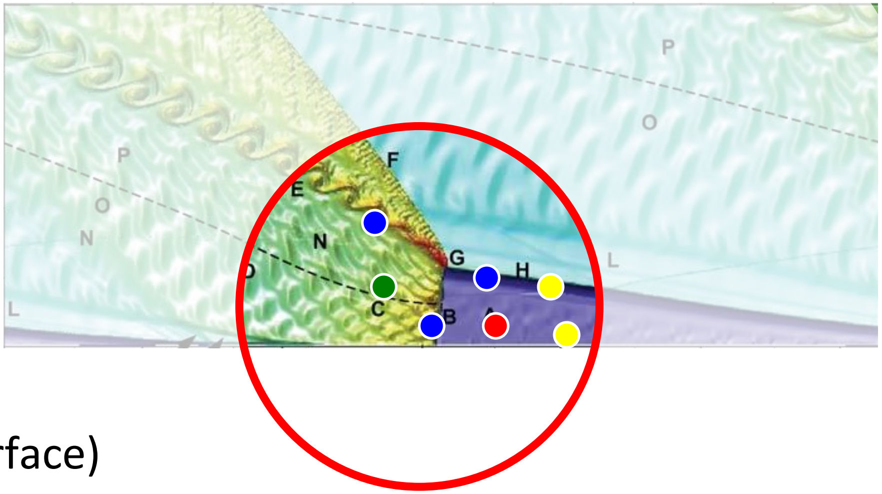
- Detonation initiation and sustainment
- Produce and maintain pressure gain
- Injector design
  - Mixing, minimize pressure drop, prevent back-flow
- Integration with turbomachinery (compressor/turbine)
  - Unsteady operation
- (High-frequency) unsteady loads (mechanical/thermal)
- Emission (NOx,UHC) mitigation



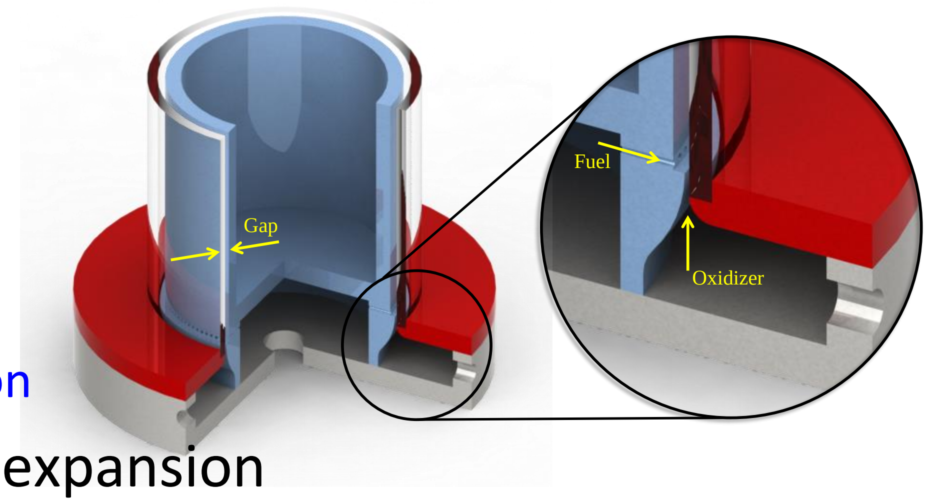
From: Falempin F., EN-AVT 2008

Non-idealities and loss of pressure gain

- Detonation non-idealities
  - – Incomplete fuel/air mixing
  - – Fuel/air charge stratification
  - – Mixture leakage (incomplete heat release)
  - – Parasitic combustion:
    - Premature ignition (e.g., burnt/unburnt interface)
    - Stabilization of deflagration (flame)
  - – Detonation-induced flow instabilities
    - Richtmyer-Meshkov (R-M) instability
    - Kelvin-Helmholtz (K-H) instability



- They lead to loss in pressure gain
  - – Linked to loss of detonation propagation

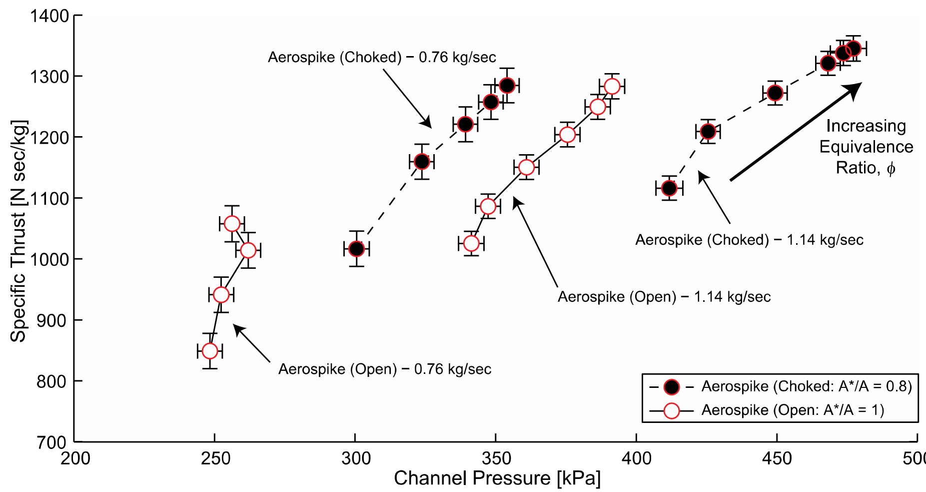


- Additional losses exist during flow expansion
  - – Secondary shock and (multiple) oblique shock
  - – Flow instabilities (e.g., K-H instability)
  - – Mixture leakage through burn/unburnt interface

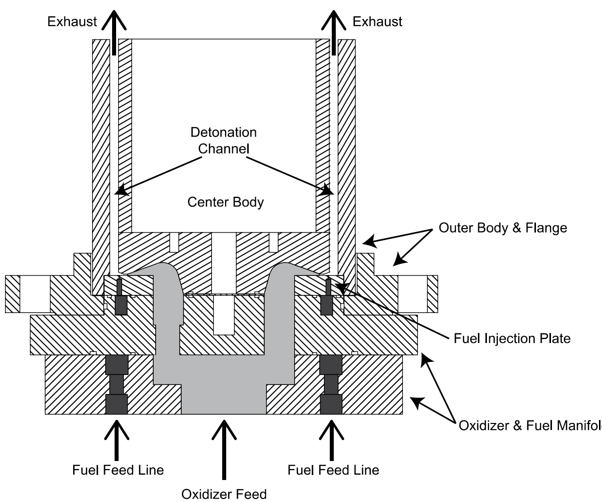
From:
(top) Nordeen et al., AIAA 2011-0803

Past/current analysis/investigation approach

- Past/current approach is based on global performance assessment
- Experimentally:
  - Global performance assessment
  - Low-fidelity and/or global metrics
    - Pressure measurements
    - Luminosity-based analysis (optical access is a challenge!)



  - Parametric study
    - Variation with flow rate, (global) equivalence ratio, fuel, pressure
    - Injector design / annulus / exhaust flowpath testing



- Prediction/computation
  - Euler solver or limited viscous effects modeling
  - One-dimension, perfect mixture
  - Single-step reaction
  - Induction-time based combustion models
  - Neglect mixing, three-dimensional viscous effects and turbulence

From: (top) Fotia et al., AIAA 2015-0631

Our approach: a multi-level physics study

Practical RDE

↓

Unit-physics decomposition

Diagnostics

- Laser-based imaging
- Mixing measurement
- Detonation structure
- Temperature and species imaging

Injection & mixing

- Free single injector
- Free multiple injection
- Confined multiple injection
- Shock-induced mixing
- DNS/LES modeling
- Experiments

Turbulence & detonations

- Linear analogue
- Detonations in stratified mixtures
- DNS/LES modeling
- Experiments

Detailed modeling

- Variable mixture ignition model
- Homogeneous reactor model with tabulated ignition times
- Non-equilibrium

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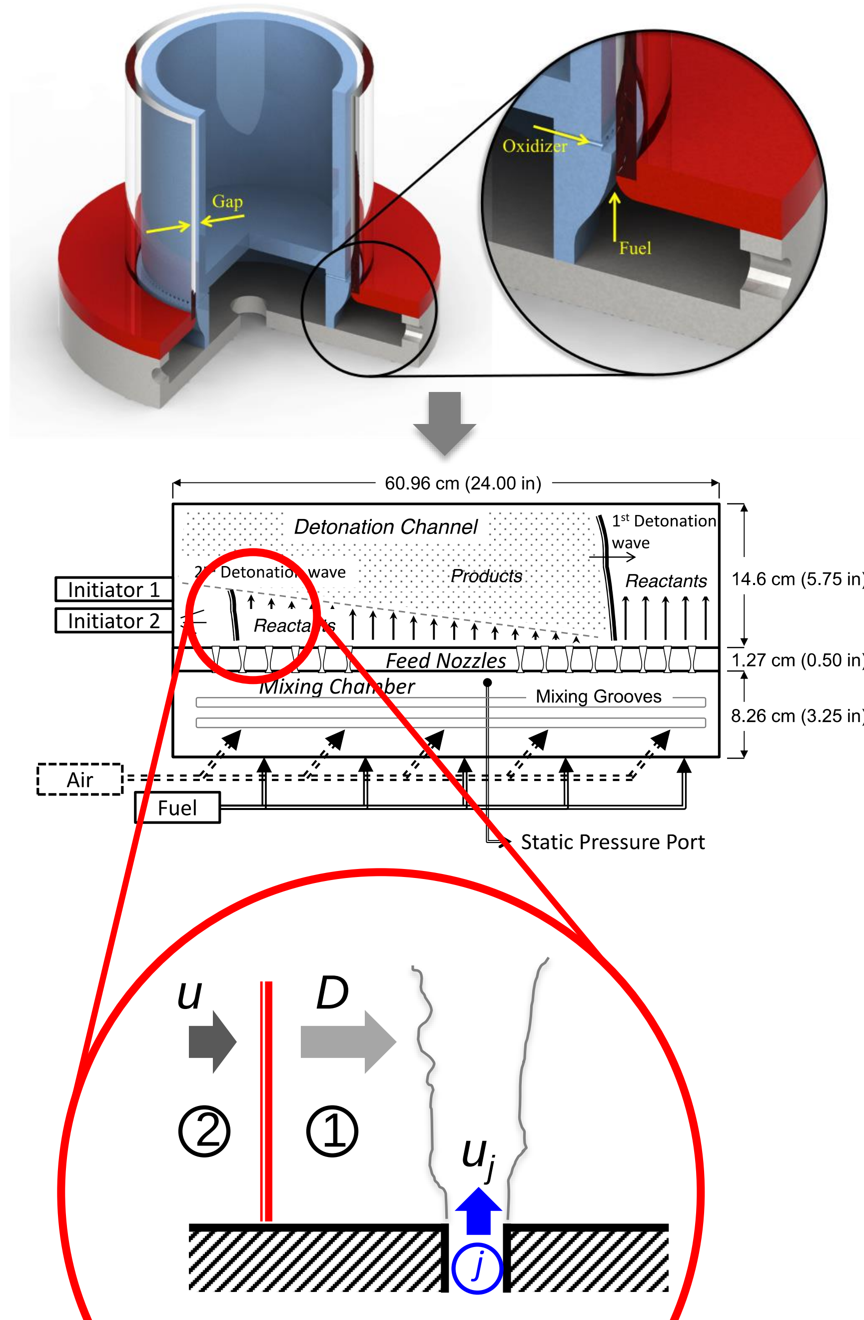
Experimental multi-level approach

RDE full system:
- Link between mixing and performance
- Design from ISSI/AFRL

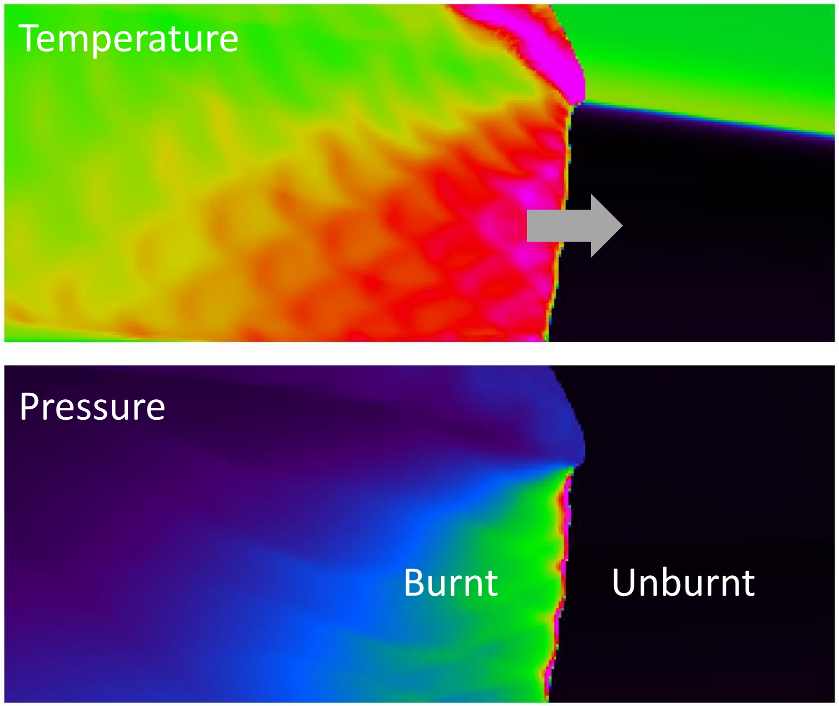
Linearized analogue:
- Detonation structure
- Detonation/turbulence interaction
- Detonation in stratified mixtures
- Design from ISSI/AFRL

Single or multiple injectors:
- Mixing studies
- Shock-induced mixing
- Our starting point

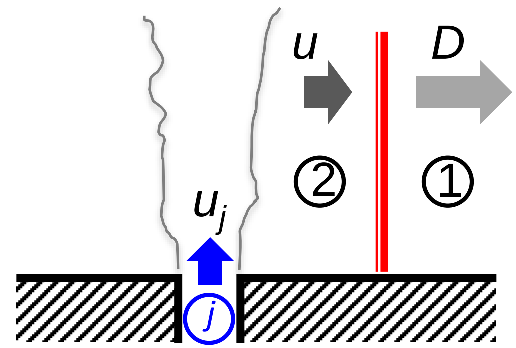


Shock-induced mixing: detonation/shock analogy

Detonation



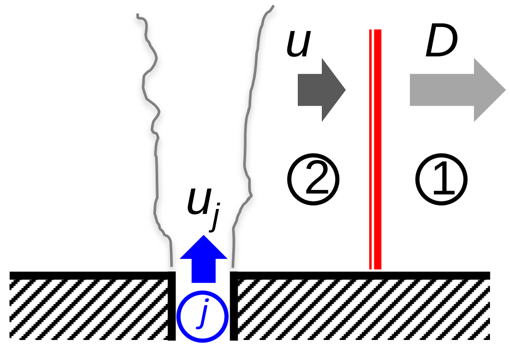
Shock analogy

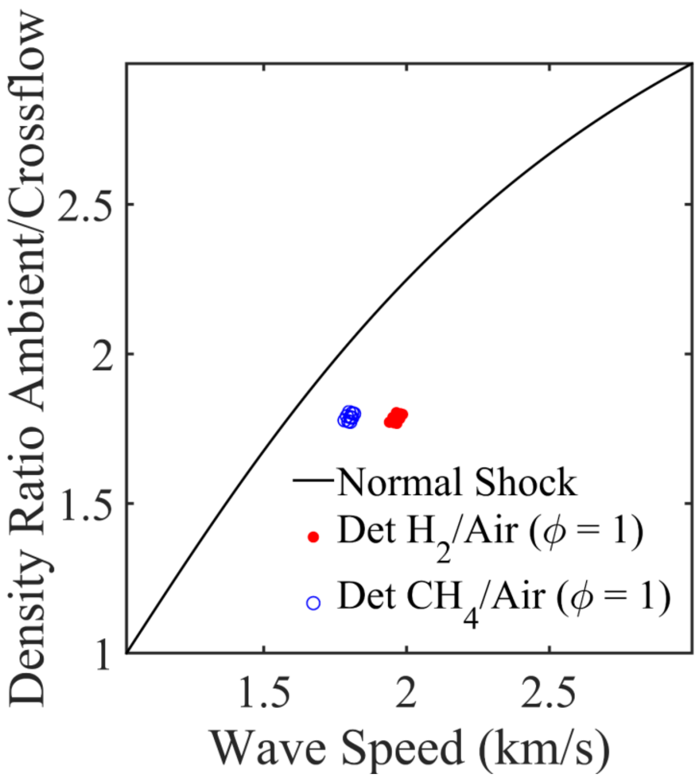


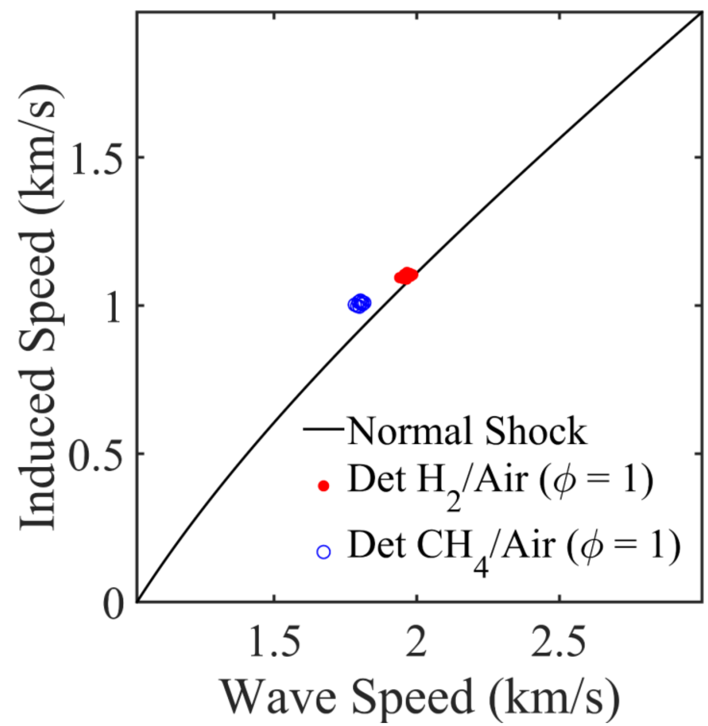
- Important parameters
  - Wave speed *D* (Mach number)
  - Jet-to-ambient (induced flow) density and velocity ratios
  - Injection pressure and configuration

From: Schwer D. A. and Kailasanath K., AIAA 2010-6880

Scaling of detonation/shock analogy







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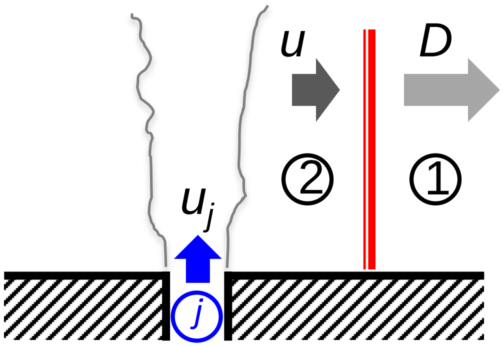
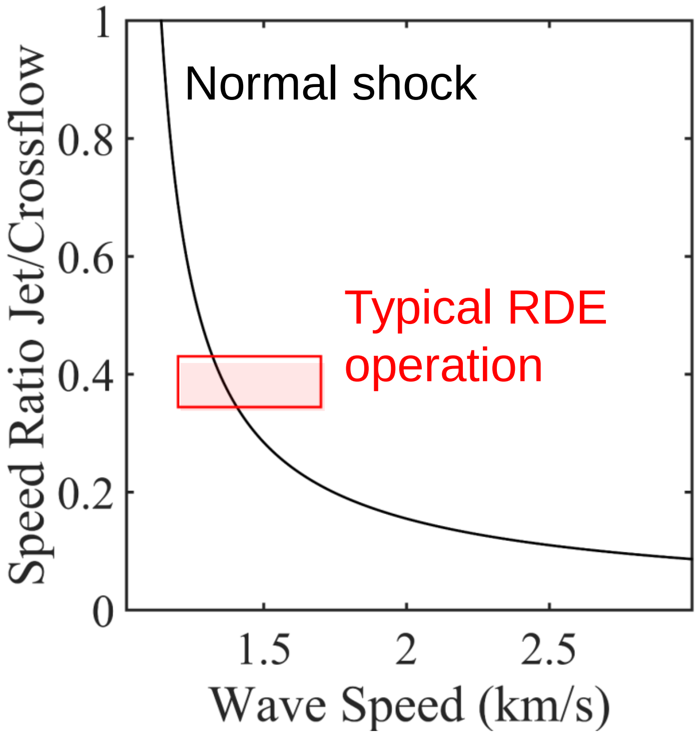
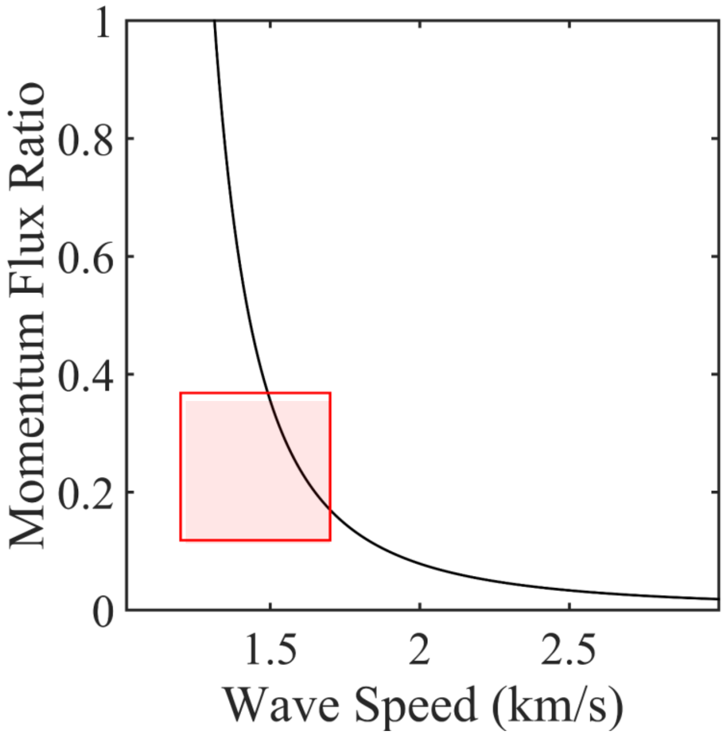


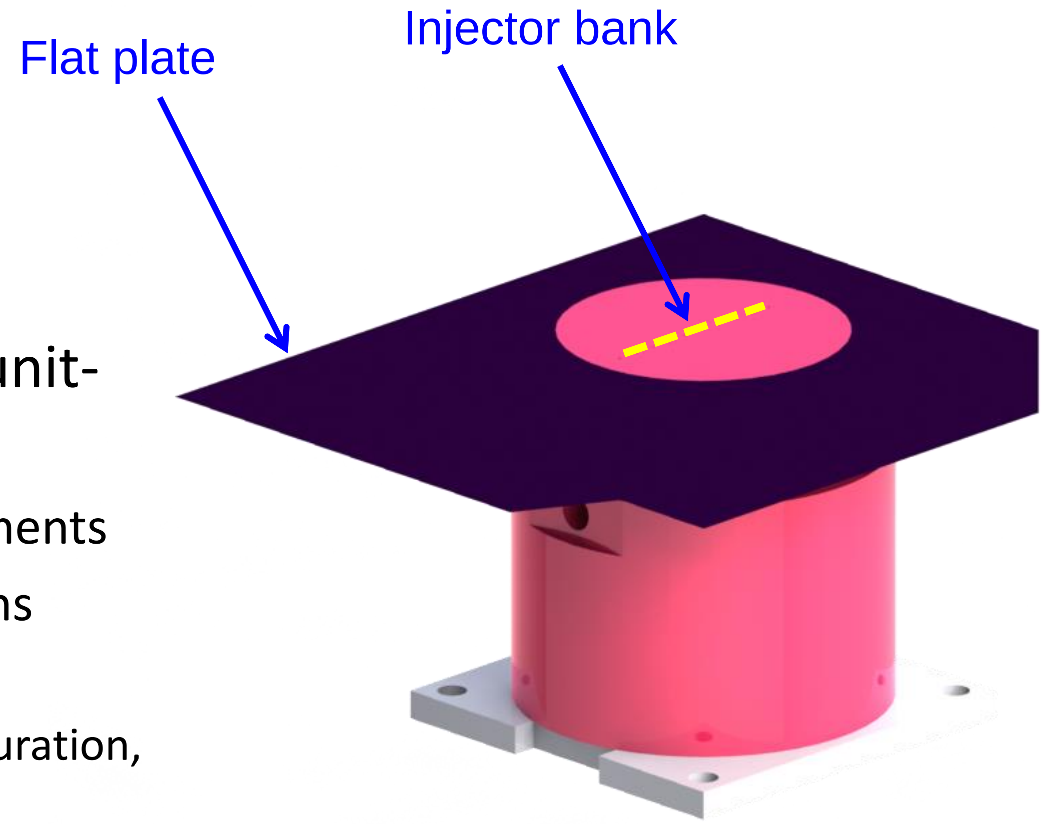




Shock-induced mixing in turbulent jets

- Flexible configuration
  - Single isolated injector
  - Multiple isolated injectors
  - Confined multiple injectors
  - Different injector configurations can be tested conveniently

- Well-suited for controlled unit-physics experiments
  - Quantitative mixing measurements
  - Flexibility in range of conditions
    - Shock strength
    - Injection details (speed, configuration, molecular weight)
  - What learnt here can be extended to the linearized RDE



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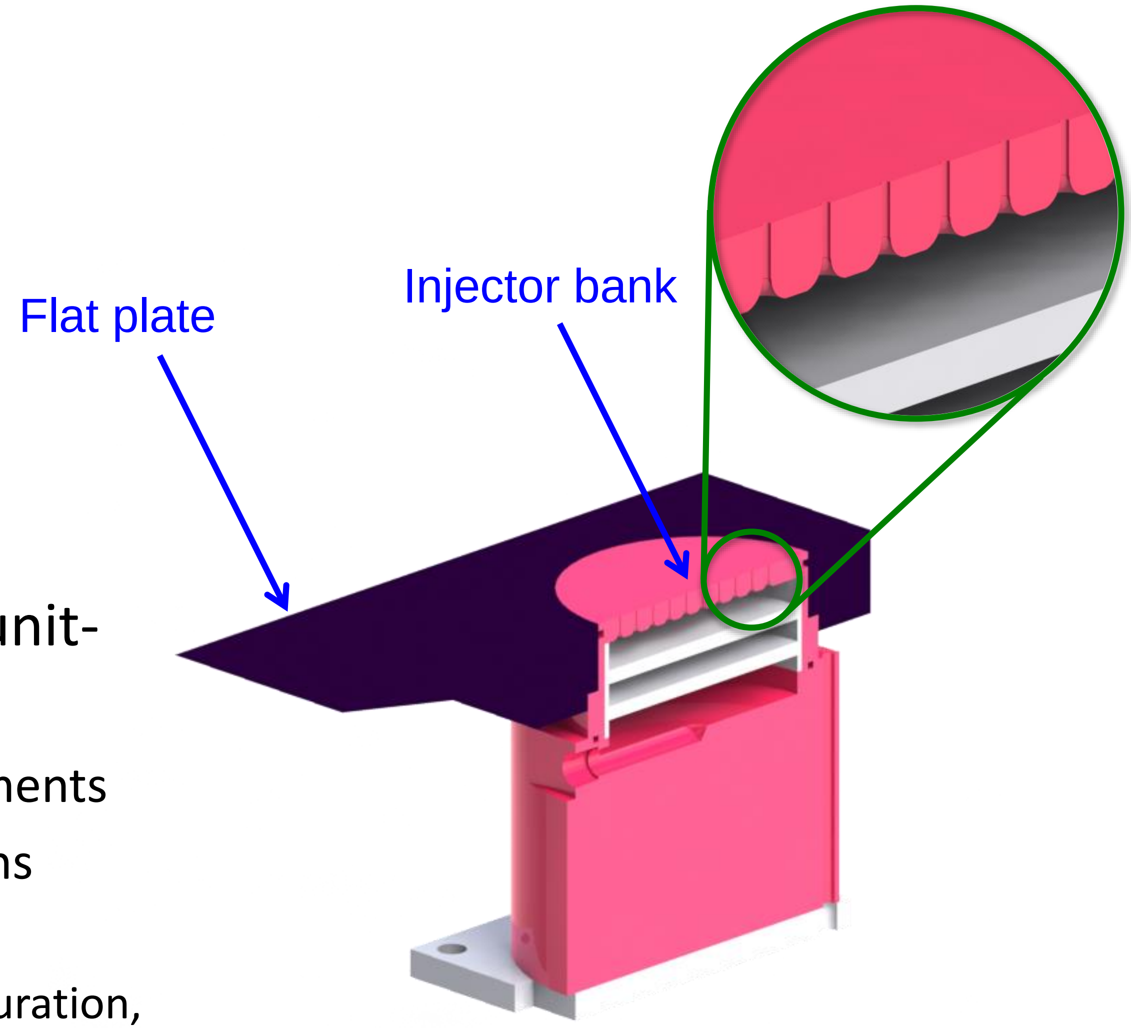

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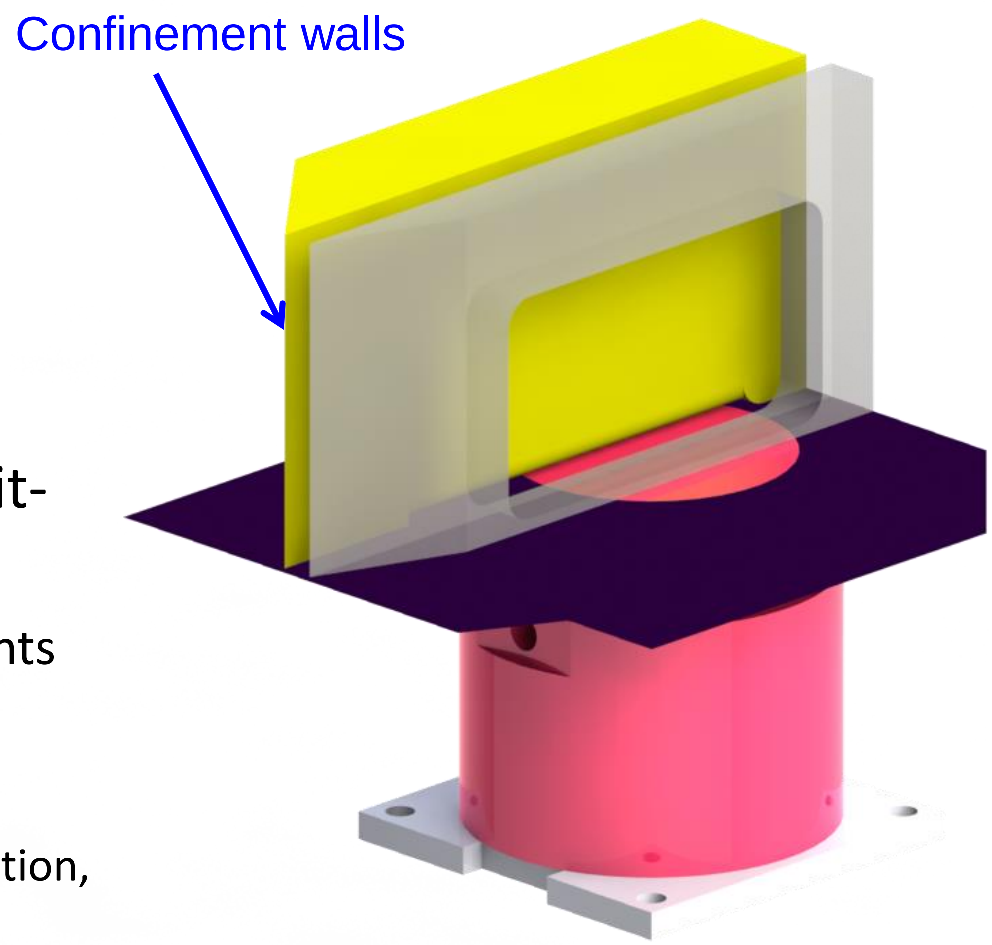

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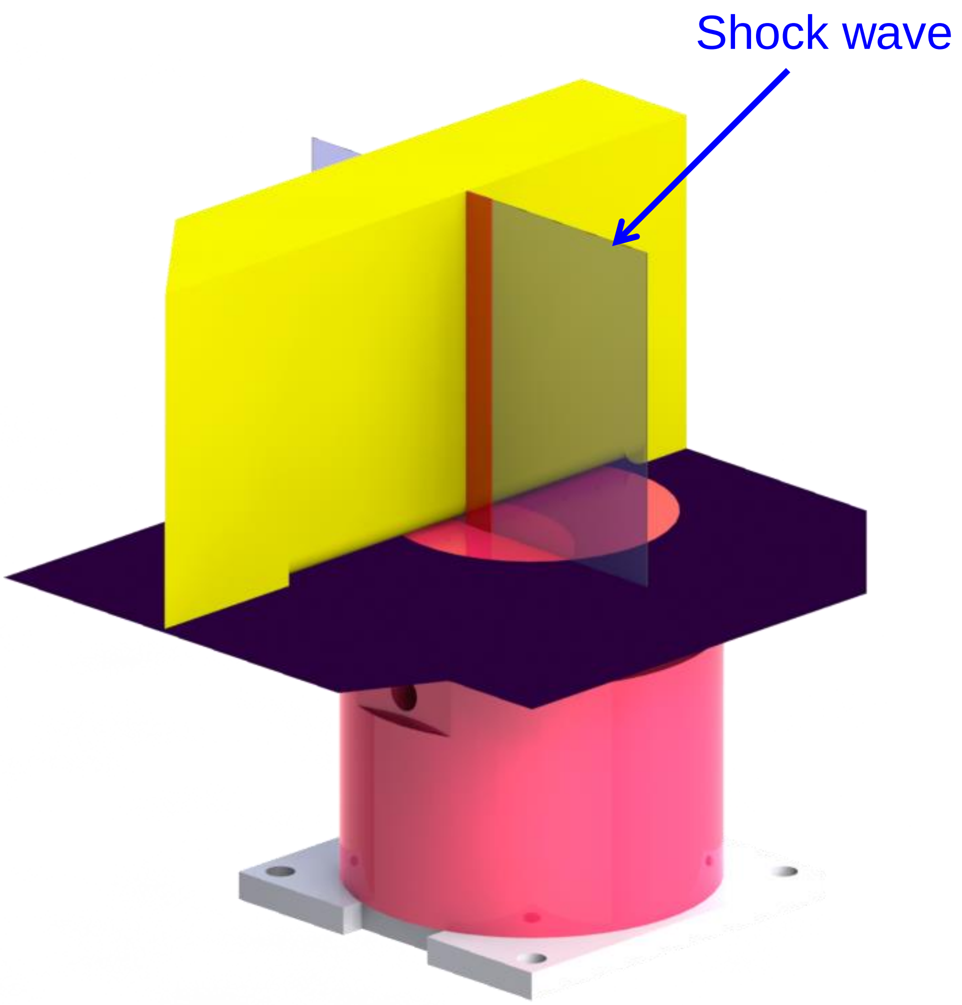

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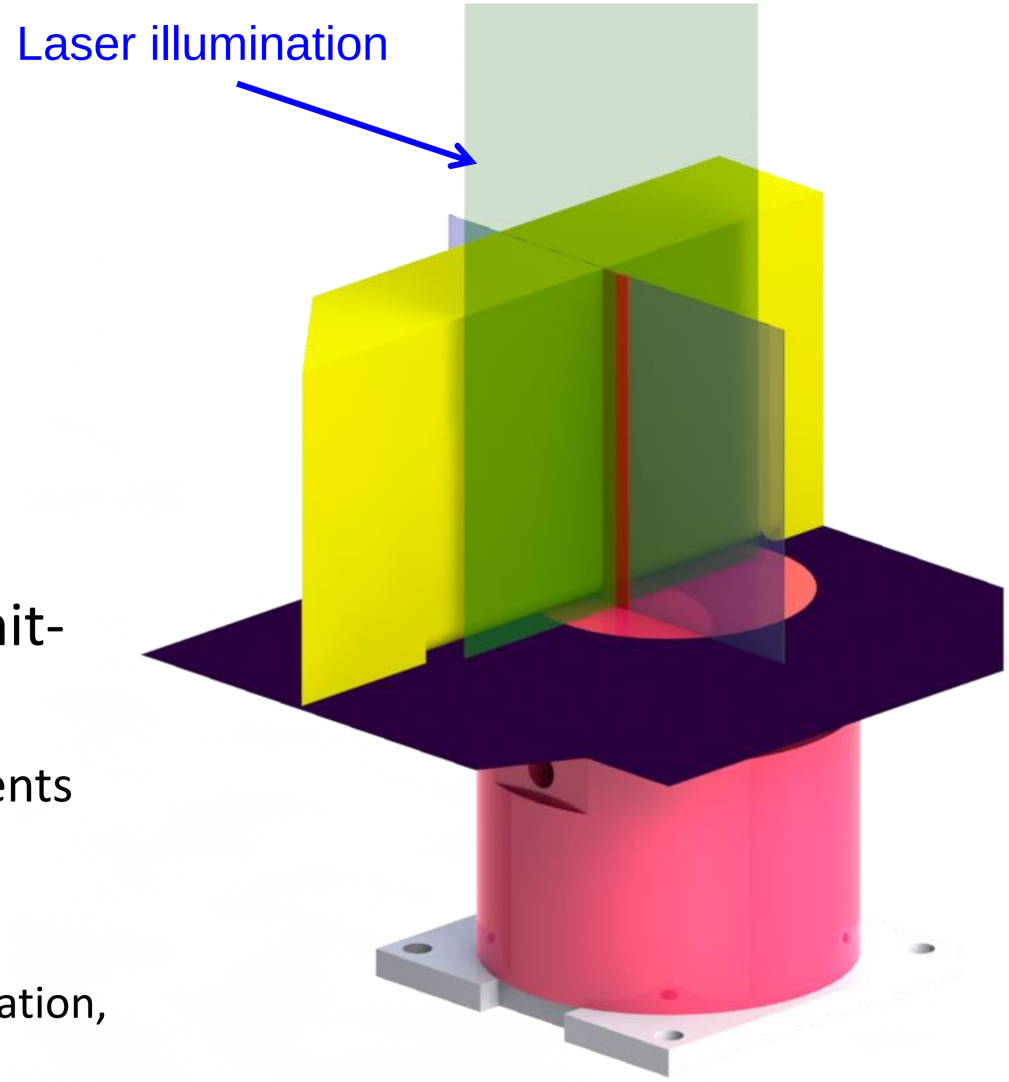

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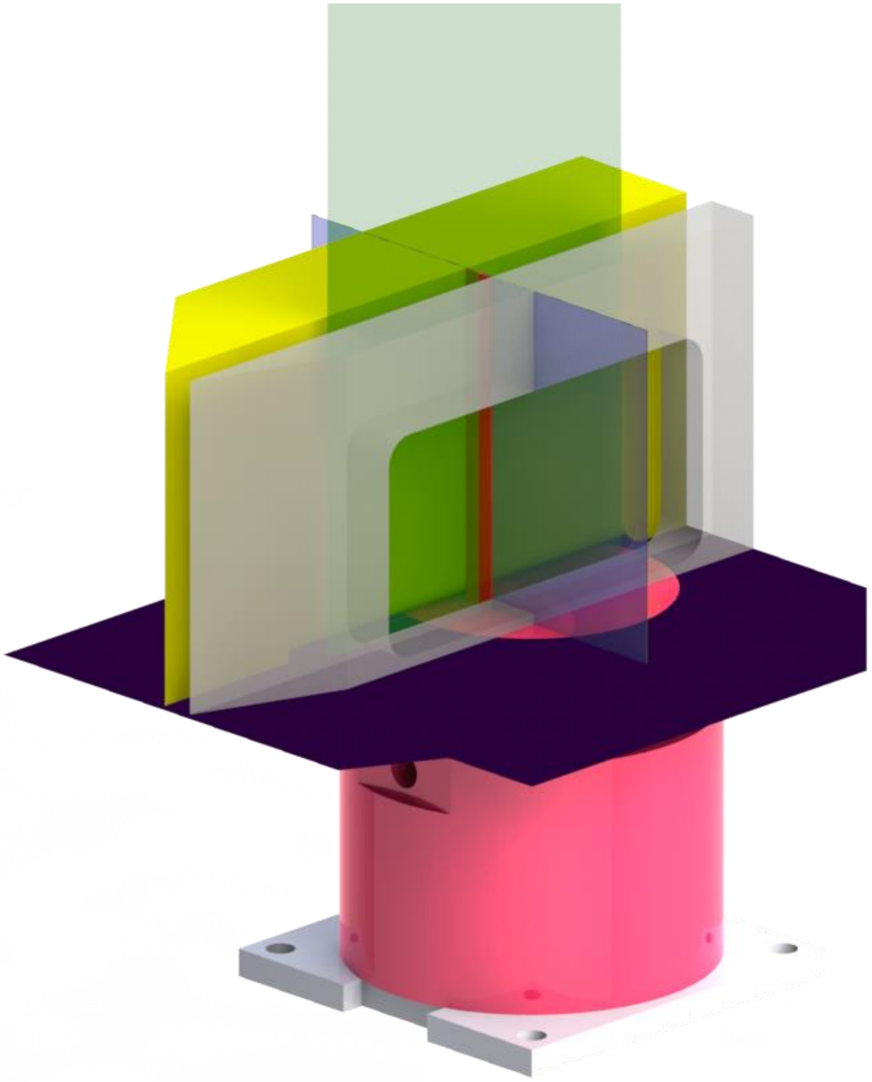

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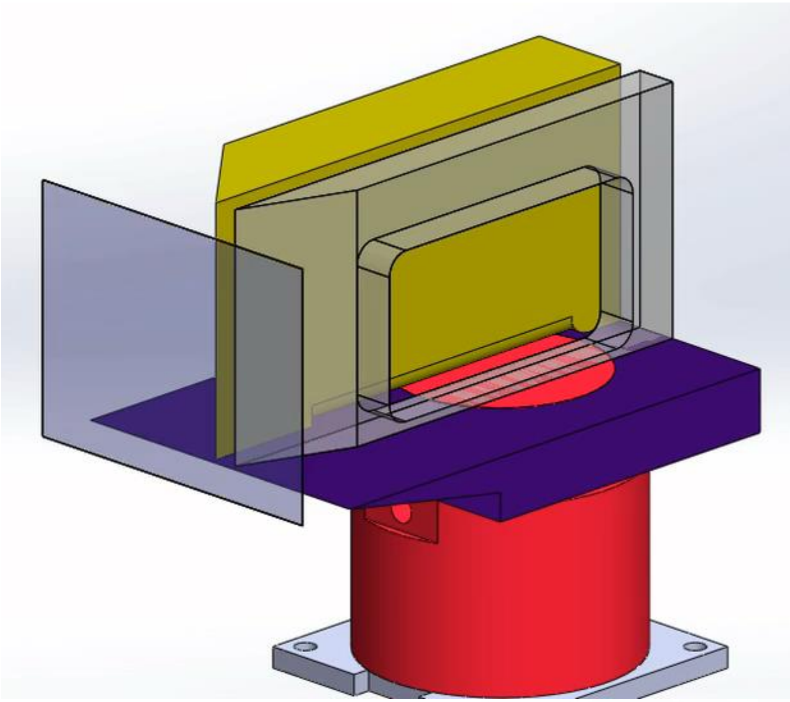
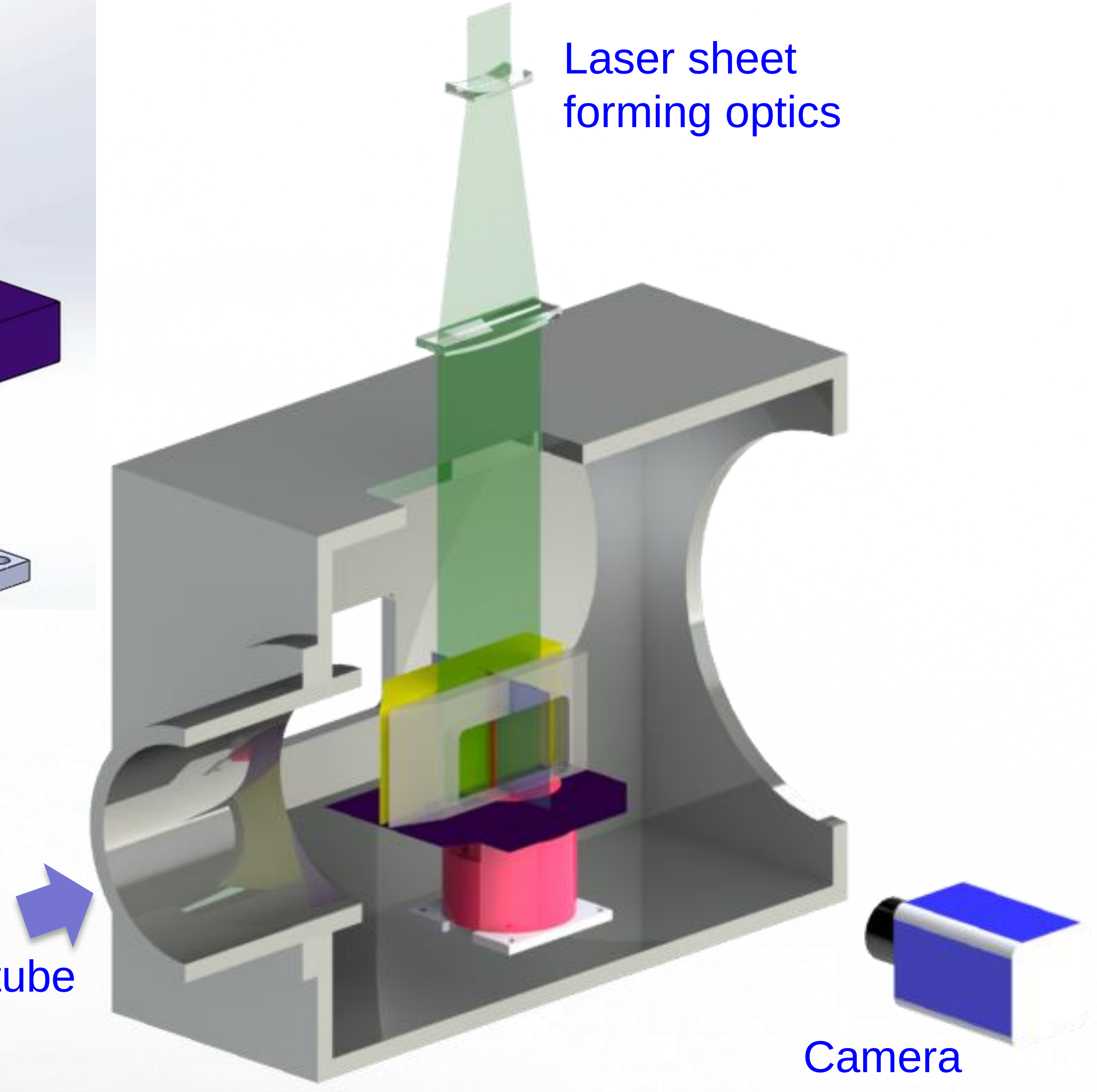
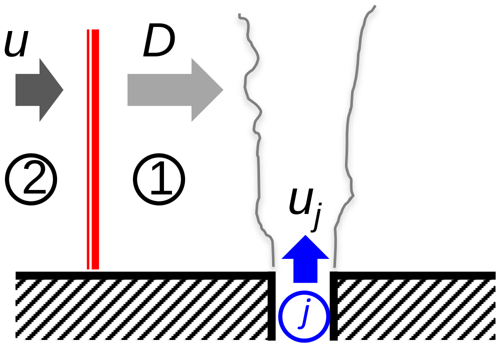
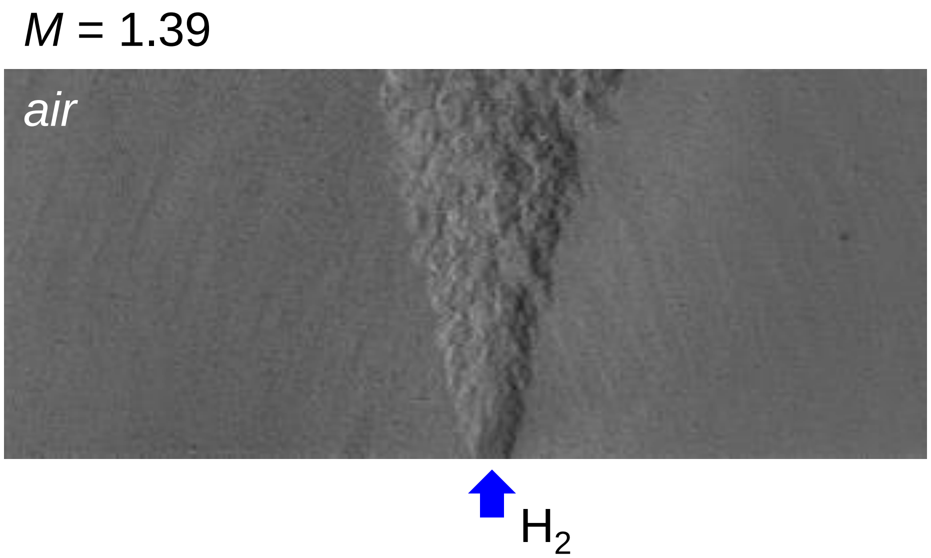




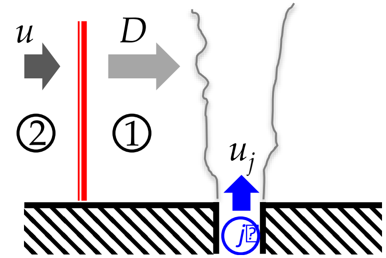
Interaction of shock wave with turbulent jet

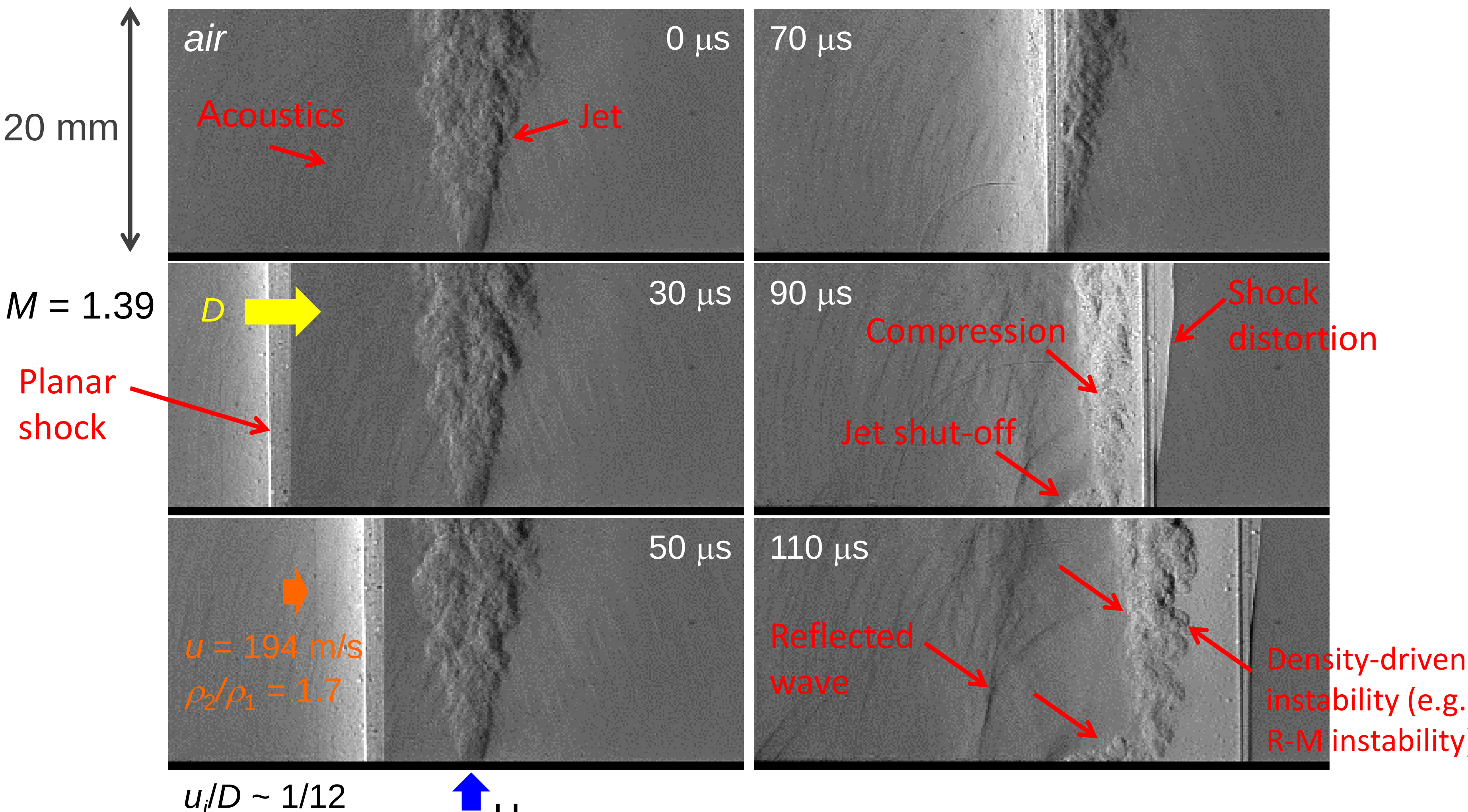




- Detonation-induced mixing analogue
- Visualization data
  - 100 kHz movie with 300 ns exposure (shock smears by 0.13 pixel)
  - Injection of H_2 into still air subject to a Mach 1.39 shock wave
  - Played back at 5 frames/second
  - Elapsed time 0.5 ms (50 frames)

Interaction of shock wave with turbulent jet

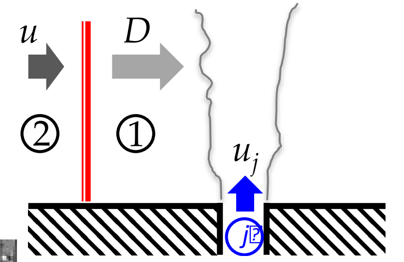


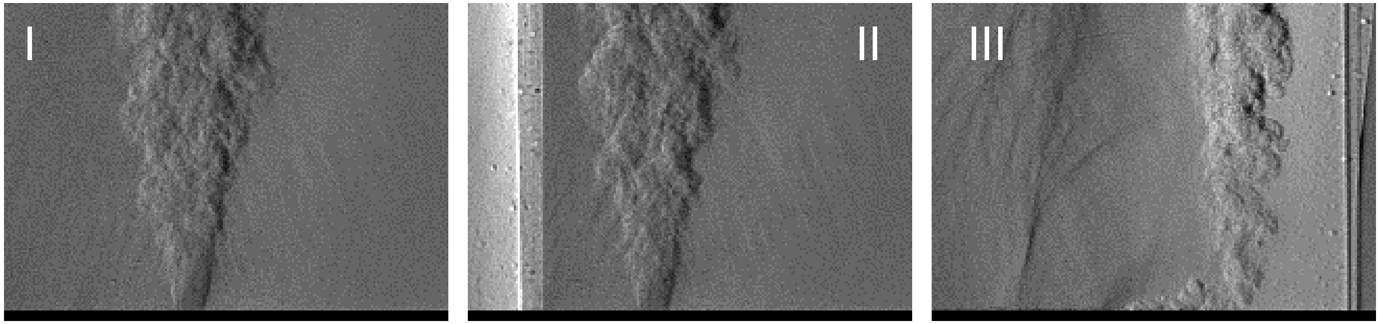


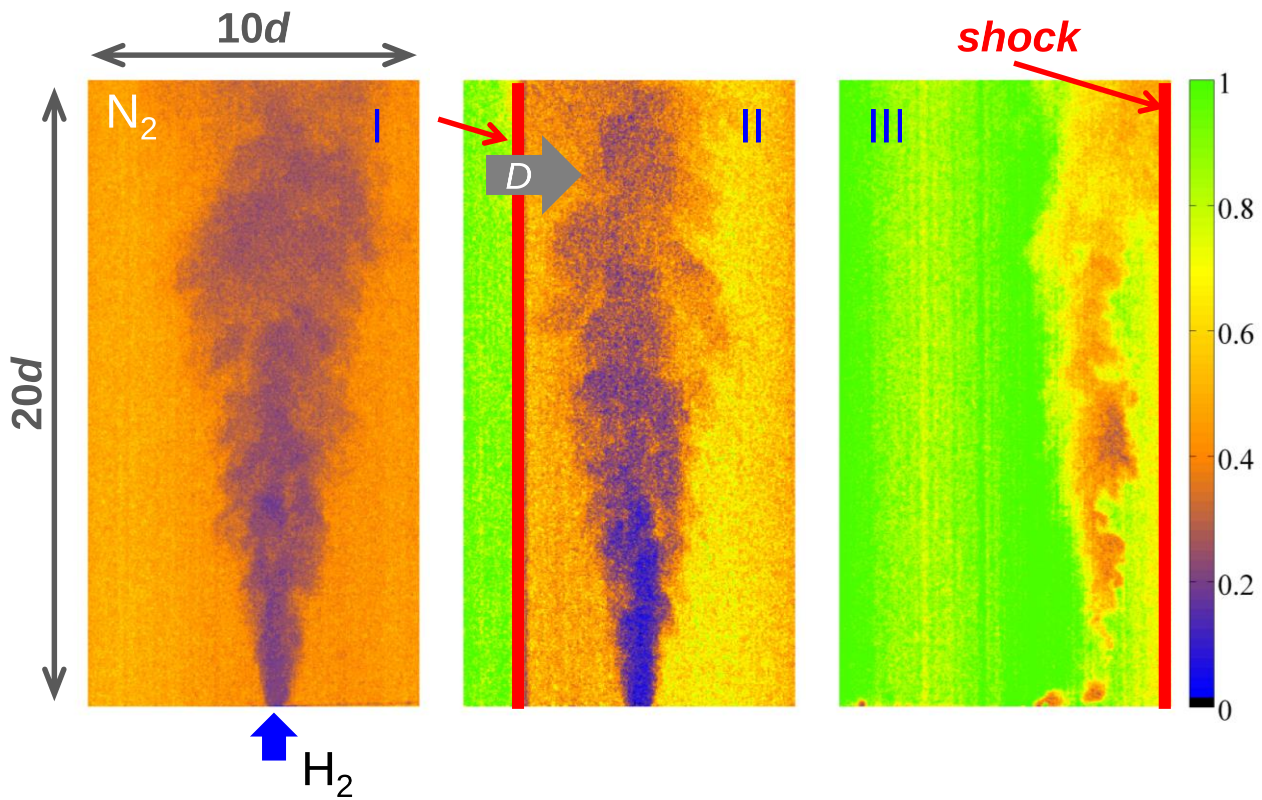
$u_j/D \sim 1/12$
$u_j/u \sim 1/5$
$\rho_j/\rho_2 \sim 1/24$

$u_j \sim 40$ m/s

Interaction of shock wave with turbulent jet (Proof-of-concept '*mixing*' measurements)







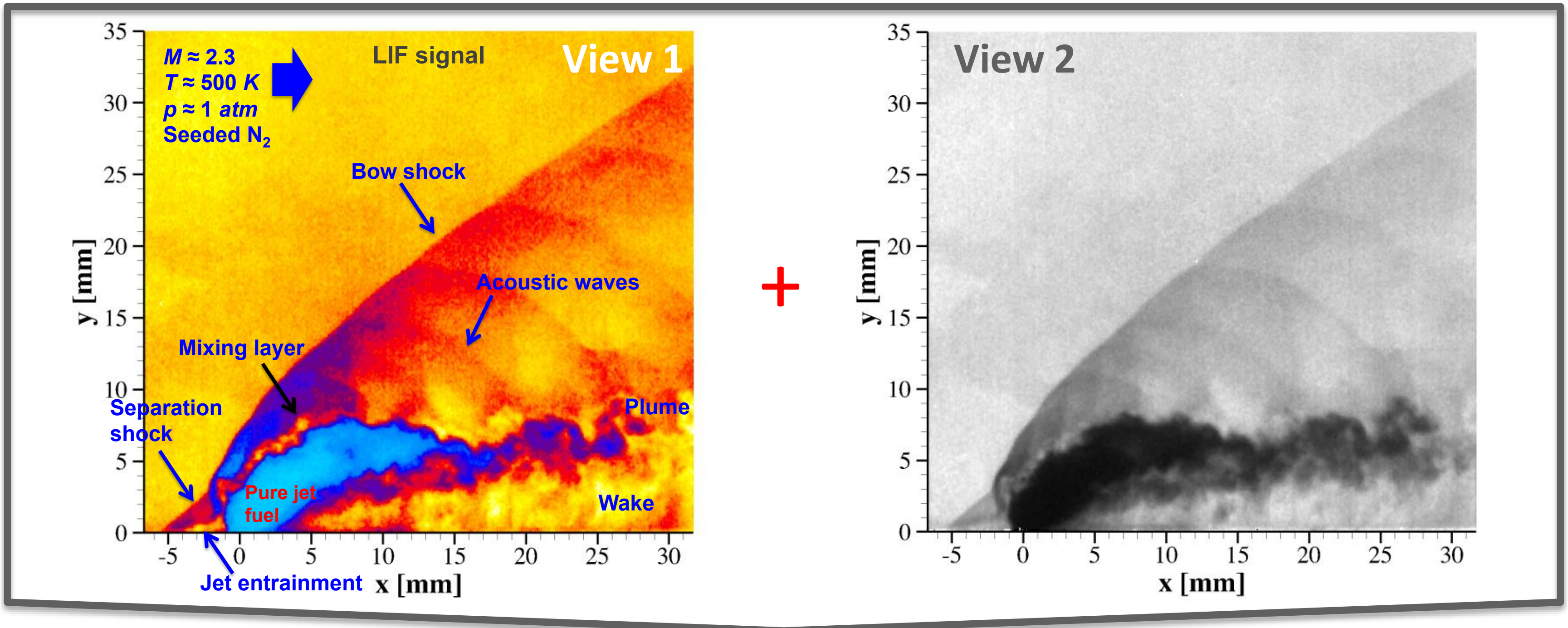
Pure ambient fluid

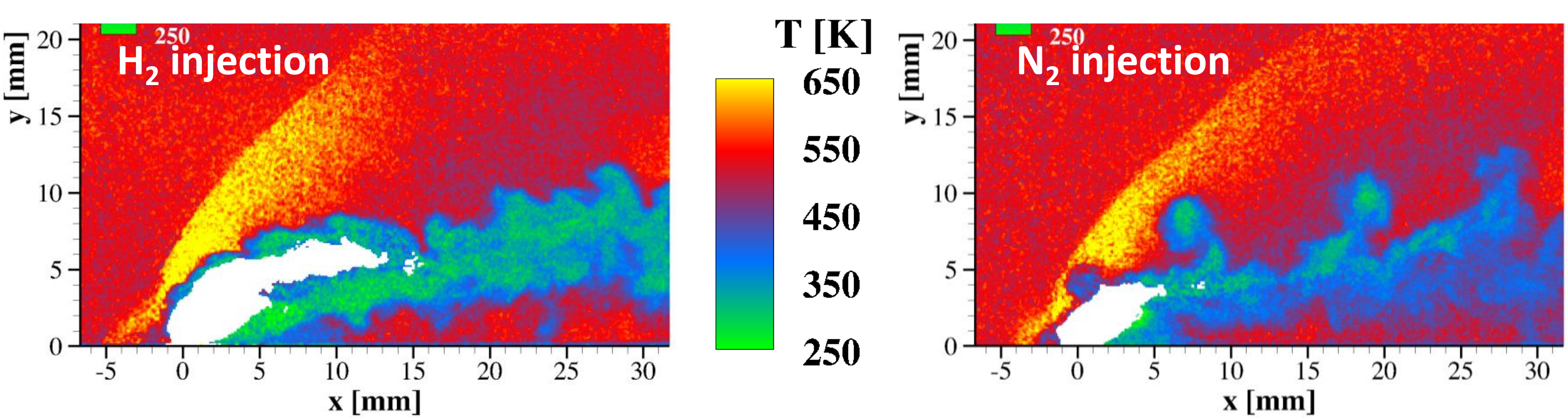
LIF signal
$S \sim f(\chi, p, T)$

Pure jet fluid

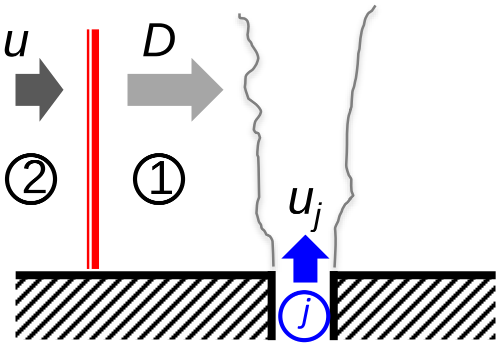
Example of diagnostic application: Making LIF measurements quantitative

Study of transverse jets in supersonic crossflow – non-reacting mixing using toluene PLIF thermometry

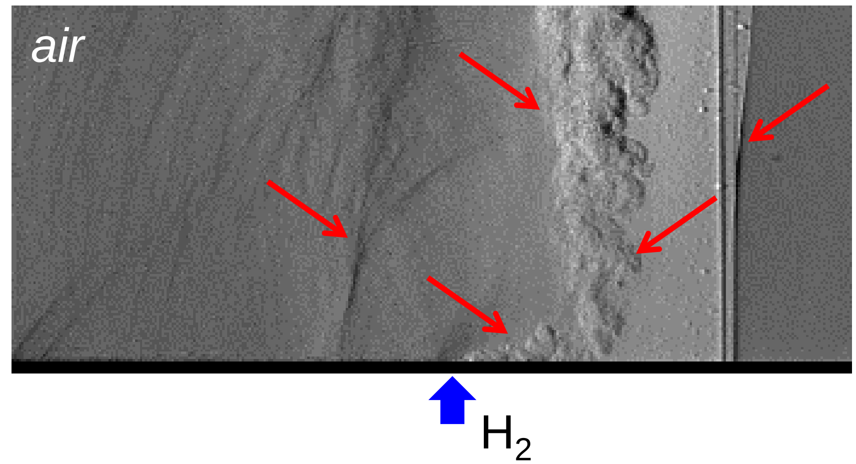




Interaction of shock wave with turbulent jet: Parametric study and outcome



M = 1.39



- Parameters to be varied
  - Shock strength (Mach #)
  - Injectant/ambient species
    - Light/heavy vs heavy/light
    - Injectant-to-ambient density and velocity ratios
    - Injection pressure ratios
  - Injection configuration
- Performance metrics
  - Degree of mixing (spatial measurement)
  - Plume shape
    - Width, corrugation, deflection
  - Length and time scales of injector response
  - Scaling with working parameters
    - Density & velocity ratios
    - Plume compression rate

Experimental multi-level approach

RDE full system:
- Link between mixing and performance
- Design from ISSI/AFRL

Linearized analogue:
- Detonation structure
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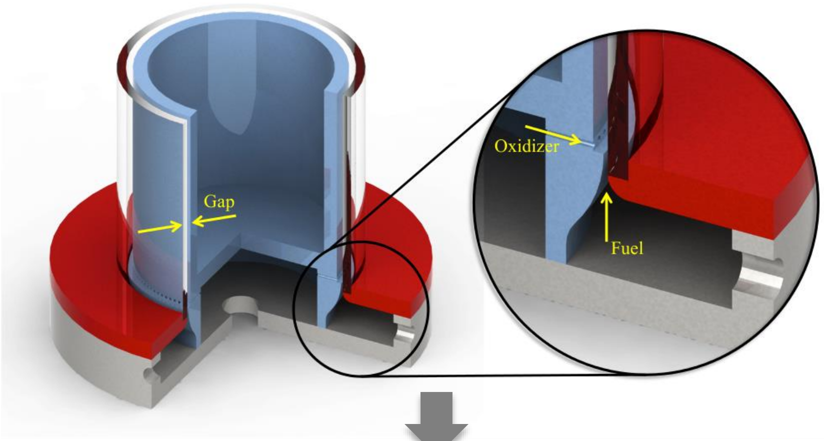
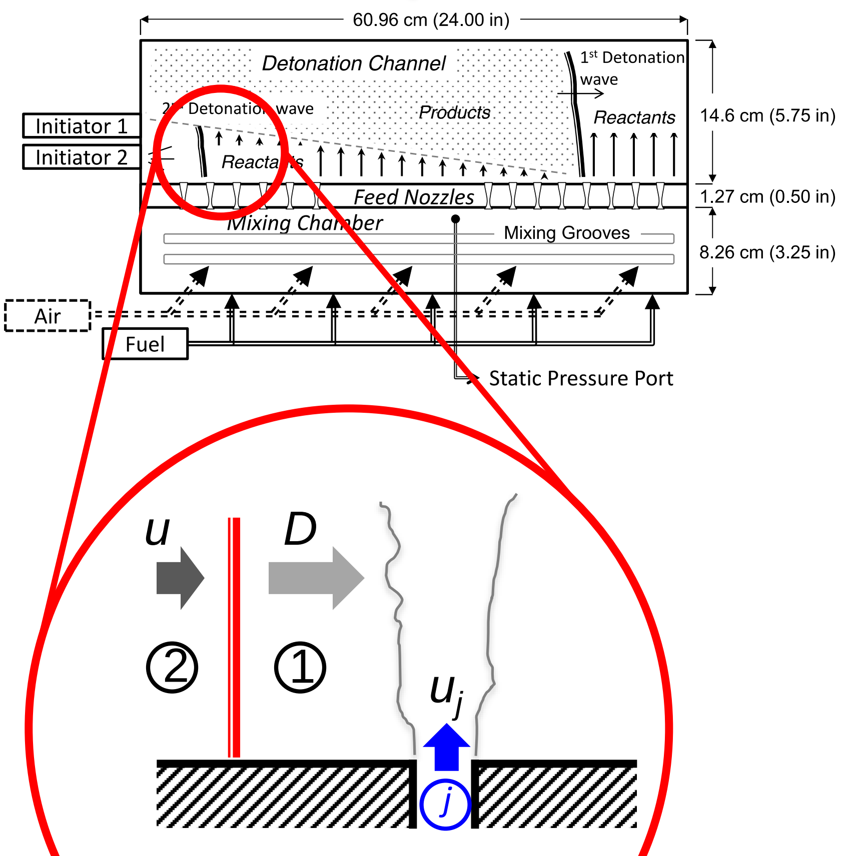
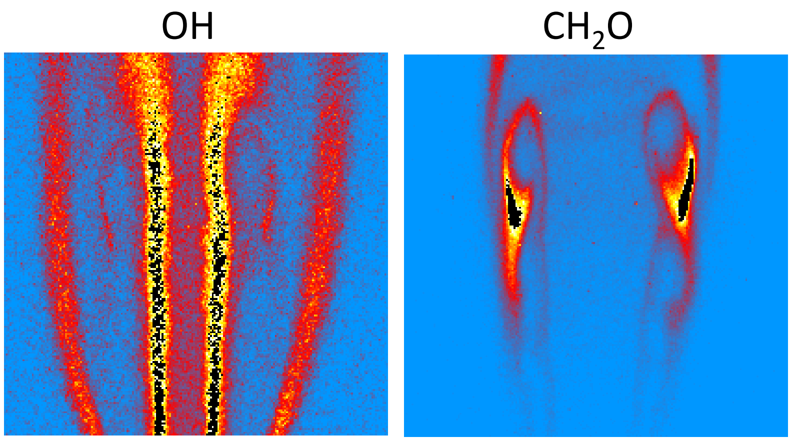




Suite of diagnostic techniques for the study of RDE physics

- Traditional techniques:
  - Pressure, heat flux, flame chemiluminescence
  - Schlieren imaging
- Laser-based imaging diagnostics:
  - Planar laser-induced fluorescence (PLIF) mixing and flame marker
  - Two-color toluene PLIF thermometry and mixing (non-reacting) imaging
  - $OH/CH_2O/CH/NO$ PLIF imaging
    - e.g., Simultaneous OH/CH_2O PLIF imaging for flame structure and heat release distribution study in premixed combustion
  - Rayleigh scattering imaging (thermometry in reacting flows)



Simultaneous OH/CH_2O PLIF imaging in inverted oxy-fuel coaxial non-premixed CH_4 flames

Next steps for experimental program

- Detailed studies of shock-induced mixing in single and multiple injector configurations
  - Design of isolated injectors completed, under fabrication
  - Lesson-learnt will be used to develop the confined injector configuration
  - Mixing measurements (temperature and injectant concentration)

- Design study of linearized RDE analogue
  - Develop in consultation with AFRL
  - Instrumented with optical access for laser diagnostics
  - Fabrication and deployment of system
  - Use what learnt from mixing measurements to link unmixedness and detonation structure
    - Speciation distribution
    - Detonation speed and height, pressure time history
    - Transition and stabilization to deflagration mechanisms

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Outline of Computational Program Discussion

- Computational platform for pressure gain combustion
- Shock-jet interaction simulations to aid experiments
- Nonequilibrium chemistry in detonations

UM Computational Program

- **Develop end-to-end simulation capability for design and optimization**
  - Computational tools
  - Models for turbulence and combustion
  - Inverse design methods
  - Fundamental chemistry analysis

- **Validation program**
  - Multi-level UM experimental data
    - Simple shock-wave interactions to realistic RDE configurations
  - External and legacy data
    - Univ. of Maryland linearized RDE experiment (Prof. Yu)
    - Other RDE projects within the UTSR program

Computational Platform

- **Computational platform should be able to handle shock-containing reacting flows in arbitrary geometries**
  - Shock-capturing
  - Resolution of turbulence structures
  - Detonation and reaction capability
  - Unstructured and adaptive grids
  - Ability to switch between LES, RANS, and Euler descriptions

- **Inverse design capabilities**
  - Adjoint tools for target-driven design modifications and optimization
  - Technology for rapid assessment of designs

Computational Tools

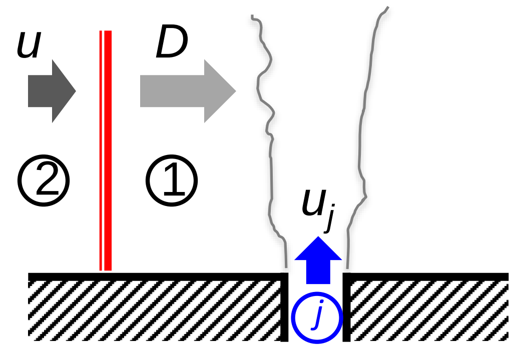
- **Open source platform**
  - Free and rapid dissemination of results and tools
  - 10K+ cores scaling
  - Adaptive meshing, adjoint tools, complex geometries, adaptive numerics
  - Integration to chemistry modules being implemented by UM
  - CAD-based meshing

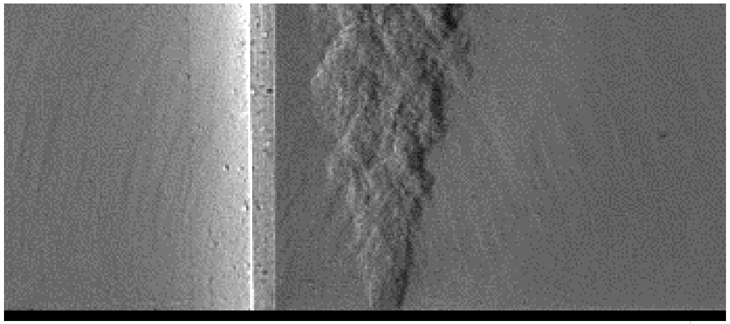
fenics project

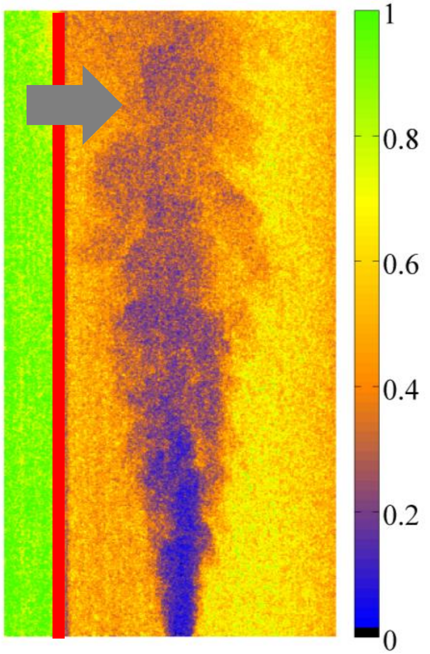
FINITE ELEMENT OPEN SOURCE SOFTWARE

DOLFIN PROGRAMMING INTERFACE

Shock-Jet Interaction

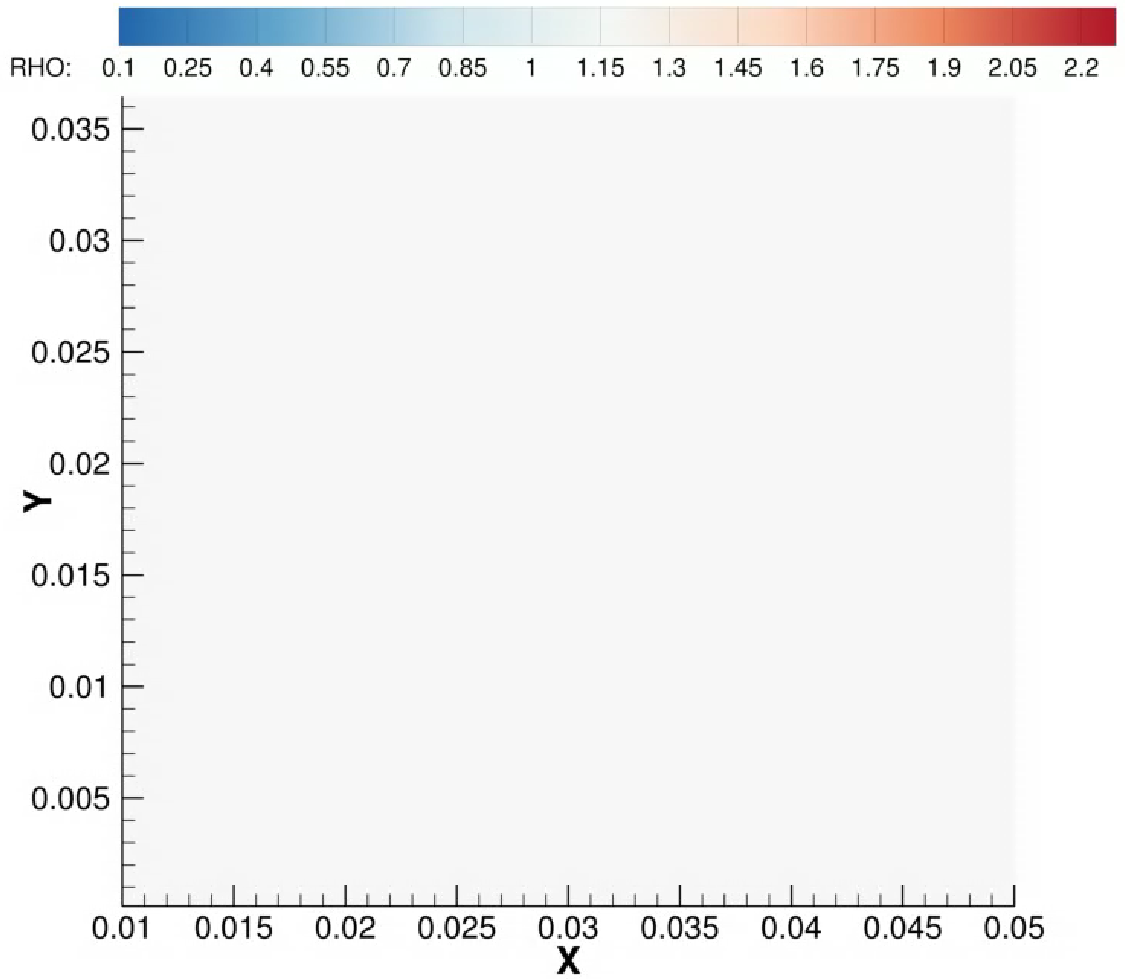






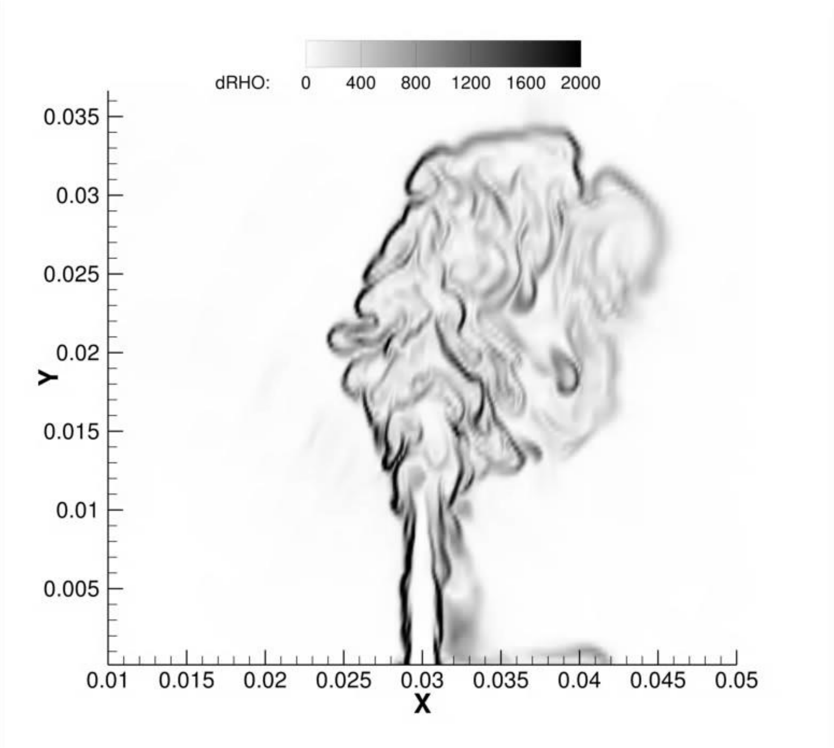
- **Simulations to aid experiments**
  - Understand turbulent jet interactions with a blast wave
- **Jet diameter of 2mm**
  - Domain (20D X 20D X 10D)
  - 256 X 128 X 128 grid points
- **LES calculations**
  - Pade' scheme
  - Artificial viscosity in near-shock region
    - Shock-sensor using pressure gradients
  - 1024 cores for 4 hours

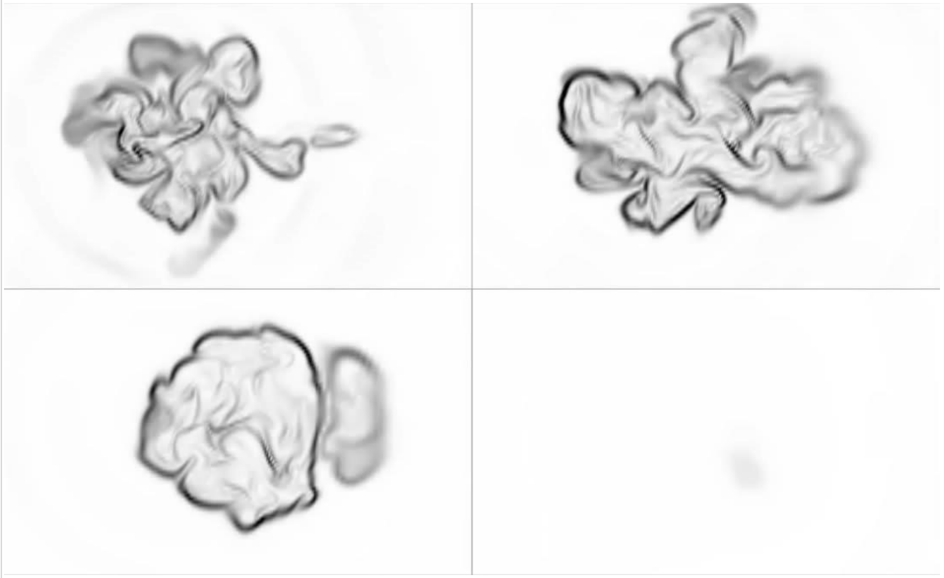
Density Evolution



Experimental Signal Reconstruction

- Numerical Schlieren





Experimental Signal Reconstruction

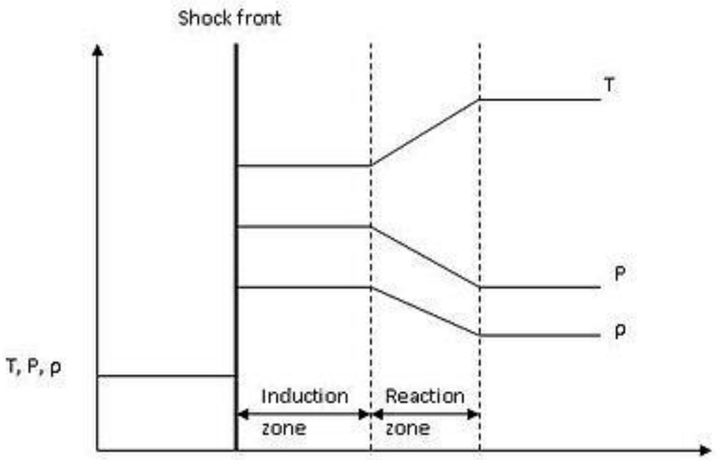
- LIF signal

Effect of Thermal Nonequilibrium

- **Shocks generate nonequilibrium**
  - Internal modes of molecular motion not in equilibrium
  - Implies that population distribution is non-Boltzmann
- **In shock-containing flows**
  - Nonequilibrium has been shown to affect chemical reactions
  - Often delays ignition
- **Detonations**
  - Conditions can support vibrational nonequilibrium
  - Thermal and rotational components equilibrate very quickly (roughly 2-10 collisions for normal conditions)

Is Nonequilibrium Important?

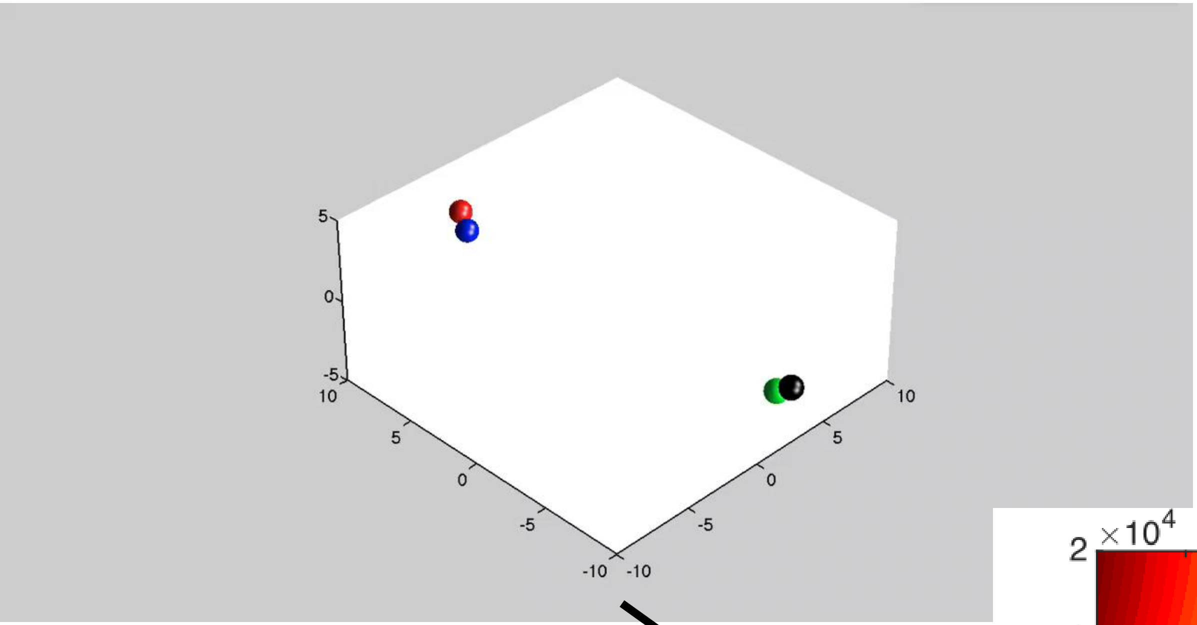
- **Question raised by NRL (Kailasnath and Schwer)**
- **No easy answer**
  - Post-detonation pressures/temperatures high
    - Relaxation time becomes very short
  - Wave structure could be affected
    - Is induction time altered?
  - Are reactions suppressed?
    - Nonequilibrium does not affect all reactions equally



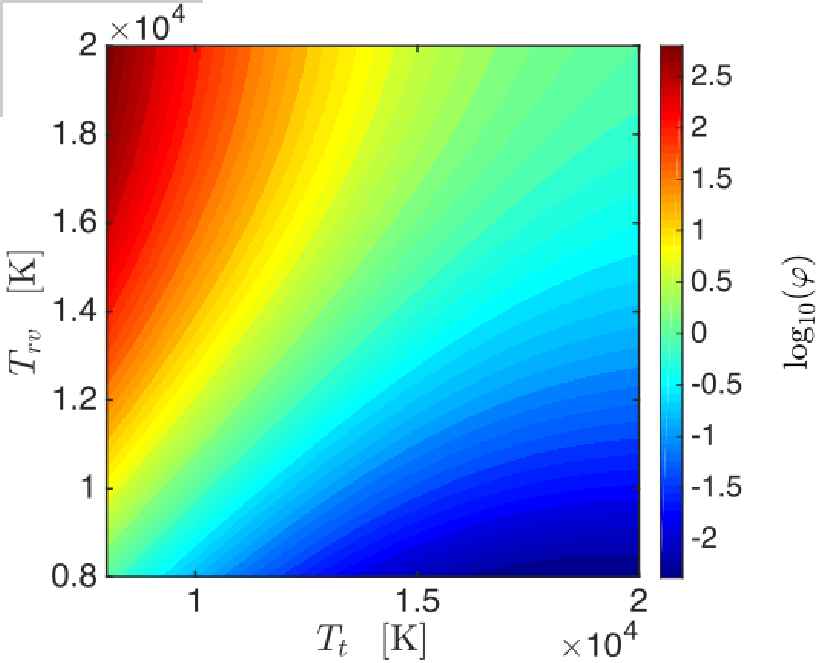
Nonequilibrium and Chemical Kinetics

- **Nonequilibrium alters chemical rates**
  - Equilibrium rates assume Boltzmann distribution
- **Difficult to obtain rates experimentally**
  - Resolving state-to-state rates is non-trivial
- **Computational chemistry**
  - Allows explicit calculation of collision cross-sections
- **UM Highly Parallel Quasi-Classical Trajectory Code**
  - Can be run on 10K+ cores (linear scaling)
  - Computes 100-1000 billion trajectories a day

QCT Trajectory



100 BILLION TRAJECTORIE S

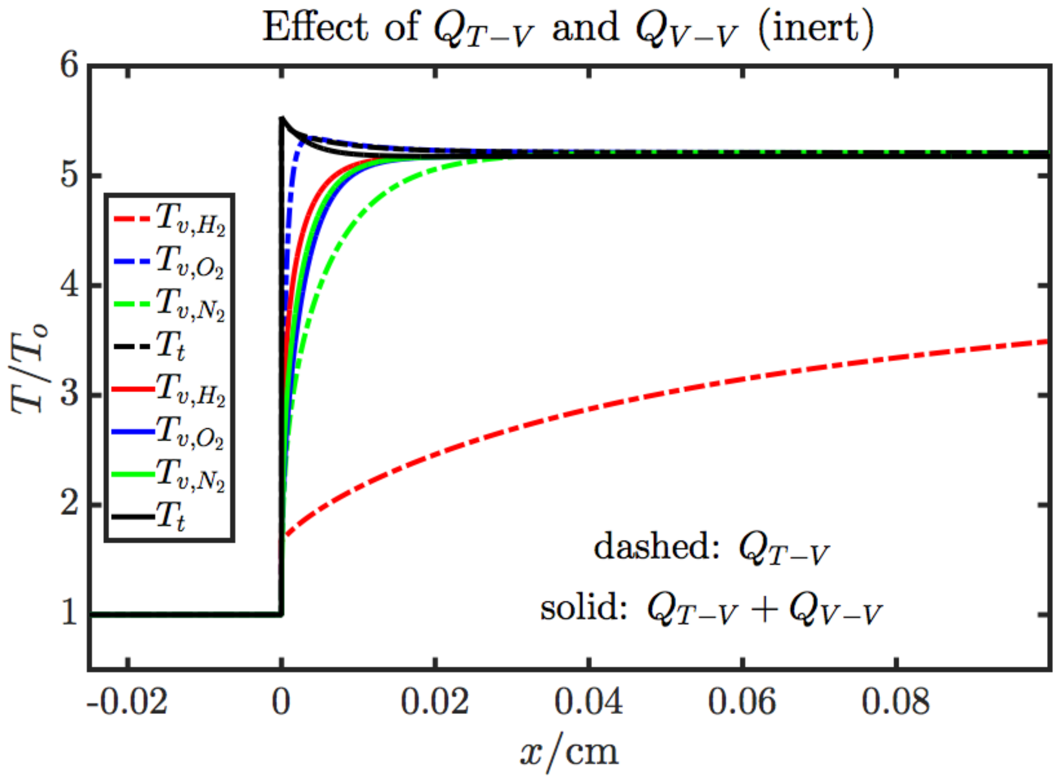


1-D Detonation Calculations

- Consider stoichiometric H2/O2/N2 system
- Ambient conditions
  - T = 298 K
  - P = 1 atm
  - M = 4.6
- 19 reaction chemical mechanism
- Each species with individual vibrational temperatures
  - Single translational and rotational temperature for all species
- Millikan and White with CVCV model used to determine T-V and V-V energy exchange rates

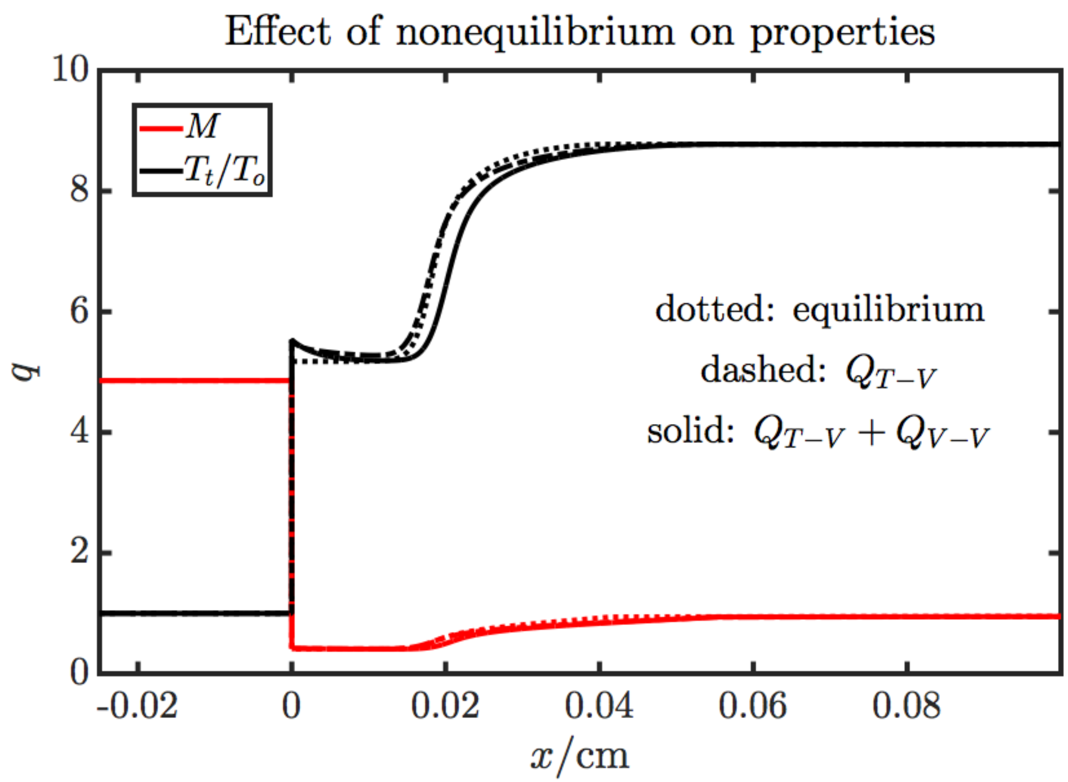
Modeling T-V and V-V energy exchange

- **Inert simulation shows relaxation of T_v back to equilibrium**
  - T-V timescale is dependent on species (H_2 relaxes slowly)
  - V-V energy exchange "averages" the vibrational relaxation time, so that each species relaxes at approximately the same rate



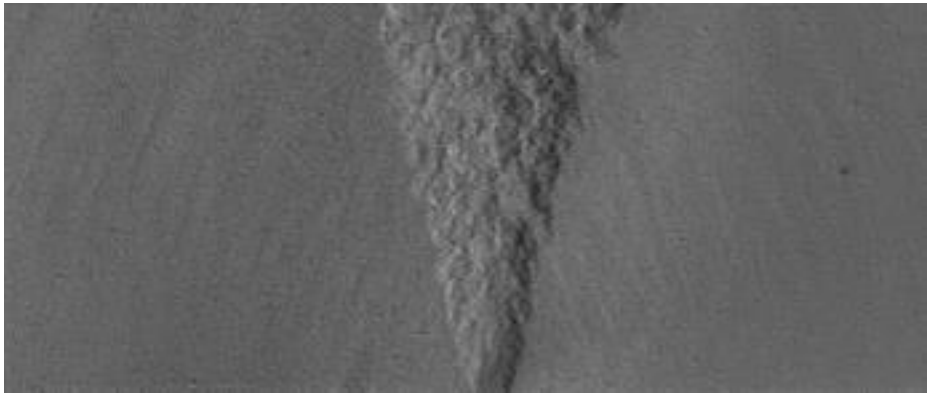
Effect of Nonequilibrium

- Nonequilibrium delays reactions
- Slight increase in induction time
- Strong H_2 nonequilibrium even post detonation



Next Steps for Computational Program

- **Start the FENICS solver development**
  - Graduate student preparing initial test version for shock-containing flows
  - Adjoint-enabled
- **Detonation simulations for linearized RDEs**
  - Solver being prepared to run anticipated experimental test conditions
  - Will consult with AFRL and NRL to determine appropriate configurations
- **Nonequilibrium effects**
  - Develop models for induction time
- **Combustion model development**
  - Use detonation DNS calculations to determine the appropriate model structure



Questions?