RA2-FA3: Characterize and Predict Physical/Chemical Effects in Turbulent Environments

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MSEE

MATERIALS SCIENCE IN
EXTREME ENVIRONMENTS
UNIVERSITY RESEARCH ALLIANCE

Scientific Drivers

SCIENTIFIC DRIVERS:

- Investigate turbulence-chemistry interaction effects on simulant-RM destruction
- Develop validated predictive tools using joint experimental-numerical approach
- Apply simulation tools with inverse UQ to large-scale, long-time afterburning

Thrust 1: EXPERIMENTAL CHARACTERIZATION

TURBULENCE
Large scale structures; mixing rates

THERMOCHEMICAL STATE SPACE
Temperature; vitiated (post-detonation) composition

MATERIALS
Simulants; addition of reactive metals

Thrust 2: MODEL DEVELOPMENT, UQ AND VALIDATION

MODEL DEVELOPMENT
Multi-scale, multi-phase modeling code LESLIE

VALIDATION
Experimental configuration; composition and time-scale effects

INVERSE-UQ ANALYSIS
Surrogate models: initial composition; temperature; mixing rates

Thrust 3: MODEL APPLICATIONS TO LARGE-SCALE DETONATIONS

FULL-FIELD DETONATION WITH LATE MIXING & COMBUSTION
Spherical charge detonation: afterburning; mixing

SIMULANT, METAL, & AEROSOL POST-DETONATION REACTIONS
Inverse UQ; sensitivity to initial conditions and residence time

CODE APPLICATION TO SCALED APPLICATIONS
Reduced kinetics for simulants & RM, aerosolized particles models

← CHEMISTRY-FLUID MECHANICAL INTERACTIONS →

Personnel

Investigators and Collaborators	Position	Institution	Workforce
Suresh Menon	**FA Coord**	**GIT**	**1 PhD*, 1 UG* (*partially shared with other projects)**
Jerry Seitzman	PI	GIT	0.85 PhD; 0.10 Res Eng.
Tim Weihs	PI	JHU	0.5 PhD
Ed Dreizin	Collaborator	NJIT	
Nick Glumac	Collaborator	UIUC	
Mark Shields	Collaborator	JHU	
Raj Sinha	Collaborator	Craft Tech	
Mark Foster	Collaborator	JHU	
Bryan Wong	Collaborator	UCR	
Mike Zachariah	Collaborator	UCR	

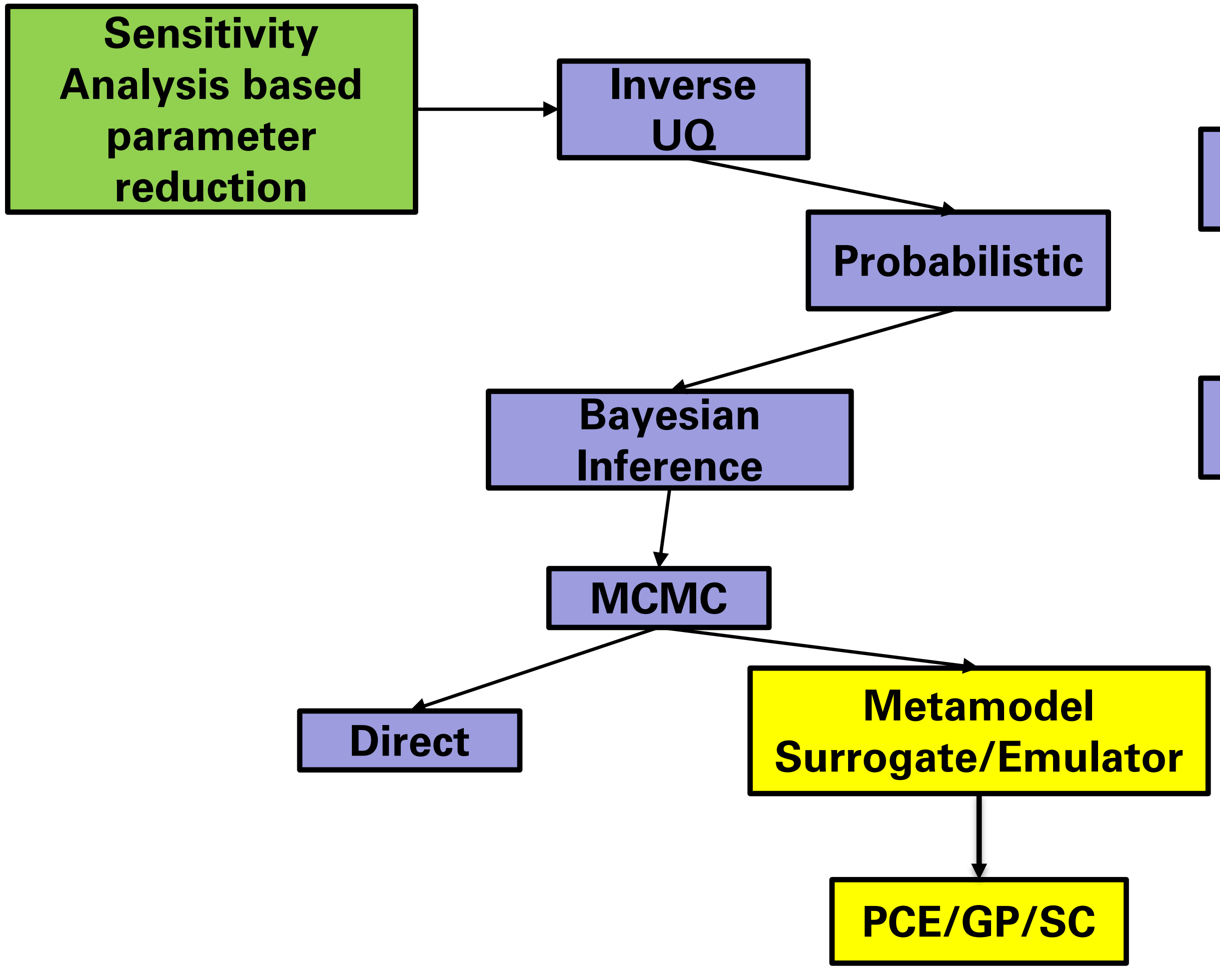
Long-term Goals and Strategies

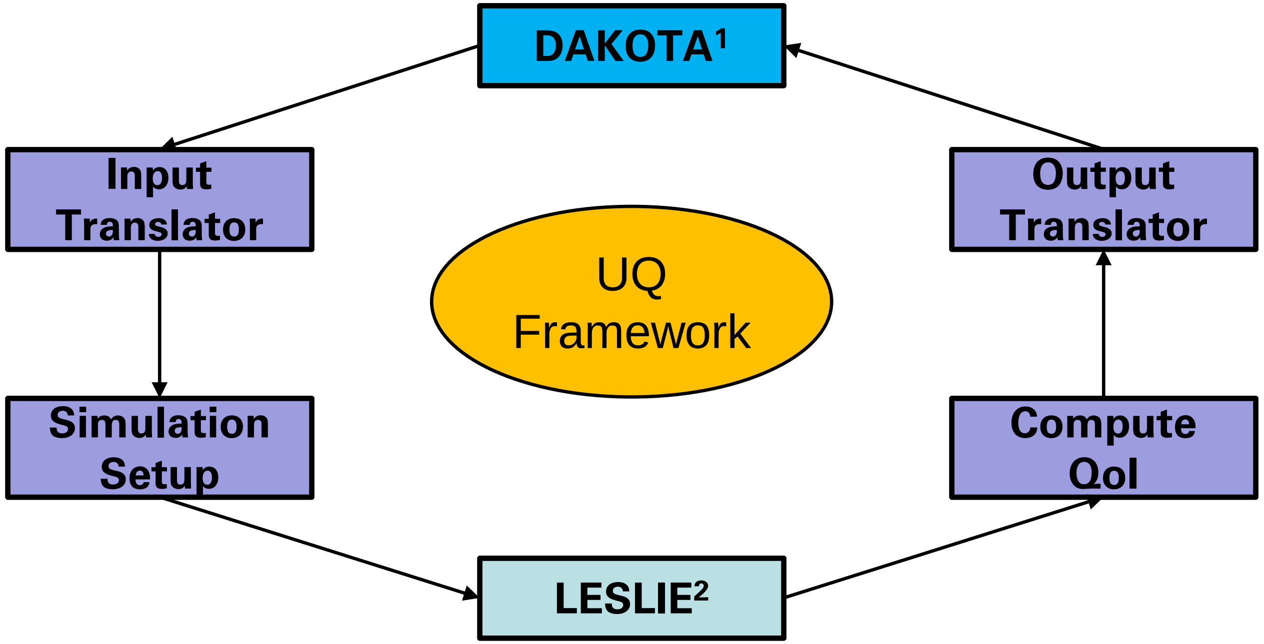
- What is the impact of turbulent mixing on simulant combustion under afterburning conditions (T, p, composition, time scale)?
- Combined experimental-numerical strategy
  - Obtain archival data for canonical problems of DTRA's relevance
  - Anchor a predictive code to these measurements (requires full 3D LES)
    - Include uncertainty quantification assessment of some of the model parameters
    - Acceleration of reduced kinetics of relevant simulant combustion (RA3-FA2)
  - Apply simulation code to study more realistic afterburning problems
    - Extend to multi-material and multi-phase turbulent mixing and combustion
    - Long term goal

IPP Goals and Strategies

- Quantify the effects of high temperature (vitiated ~1400-1800K), composition(CO_2, H_2O, etc.), residence time (1-100 ms) @ 1 atm
  - Focus on DIMP as simulant now and add metal oxides (JHU) later
  - Coordinate with RA3-FA2 for kinetics models and with RA2-FA2 for UQ
- Exp: Inclined JICF to vary residence time in the burning domain
  - Contains all features of shear layer, wake and multi-species mixing
  - Study *Re*, T, u' and composition effects on simulant combustion
  - Diagnostics (PLIF, PIV, GC, etc.) to get archival data for code validation
- CFD: Code anchored using JICF data and for various initial conditions
  - Develop reactor network ROM for rapid parametric evaluations
  - V & V with limited full 3D LES

Approaches to Perform Inverse UQ For RA3-FA2

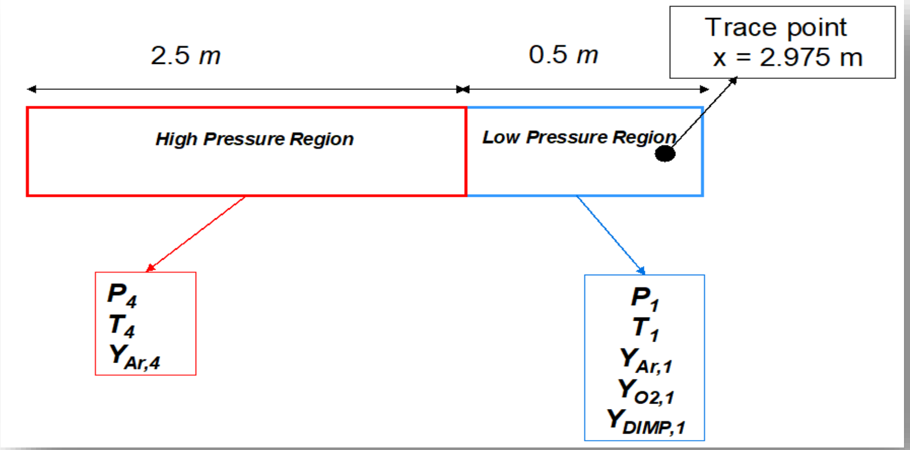


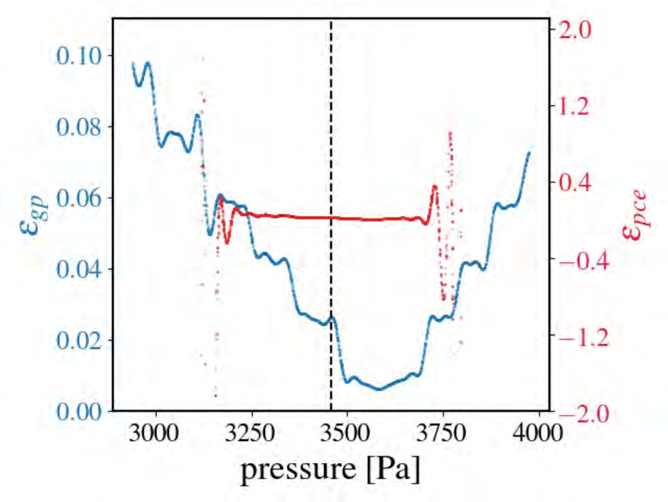


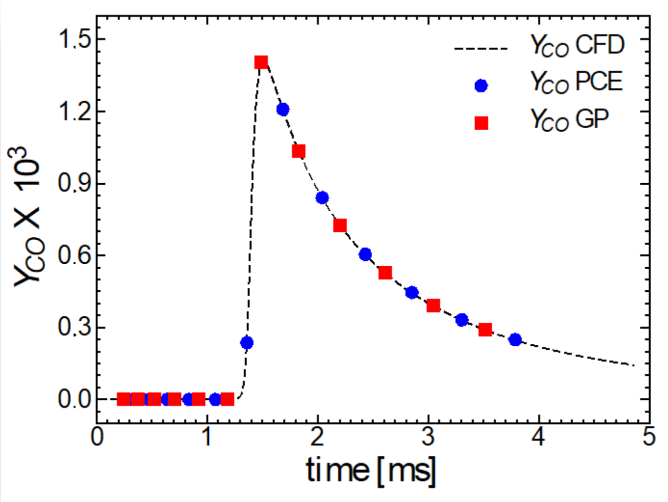
QoI: Quantities of Interest

Simulant – Kinetics Assessment (under RA3-FA2)

- DIMP: 278 species-1250 reaction mechanism reduced to 73 species and 275 reactions (2020)
- Reflected Shock Combustion in shock tube
- **Past Work:** determine posterior statistics of uncertain parameters P_1 and X_{O2_1} through surrogate models (PCE and GP) for IUQ*





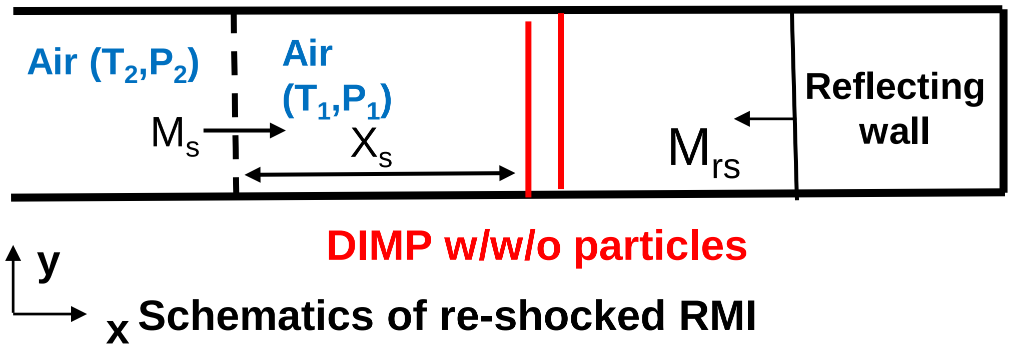


- Collaboration with RA3-FA2
  - Further Kinetics Reduction
  - Inverse UQ (IUQ) modeling
  - Shock tube data for V & V
  - Extension to two-phase (longer term)

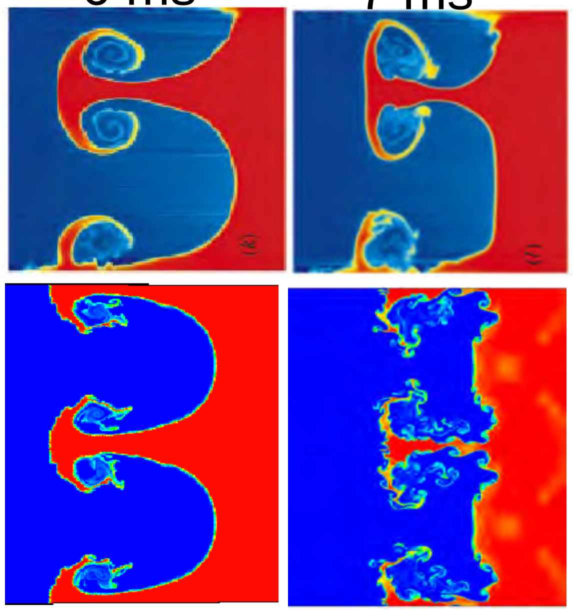
* AIAA-2020-2137

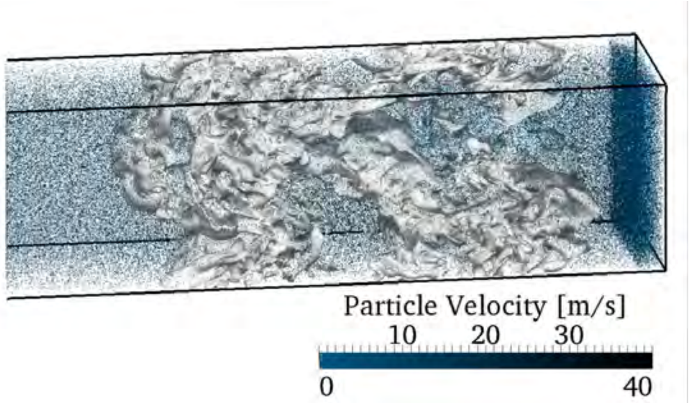
Simulant – Turbulence Assessment (under RA3-FA2)

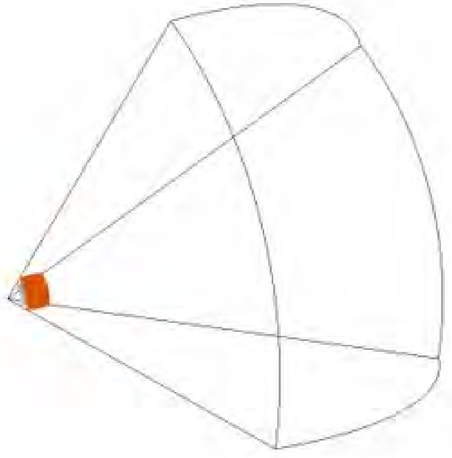
- Re-shocked RMI: a canonical problem
- Simulant curtain with and w/o metal particles
- Turbulent mixing with and w/o combustion
- Capability exists but need inputs from FA2
- Limited studies in first phase planned



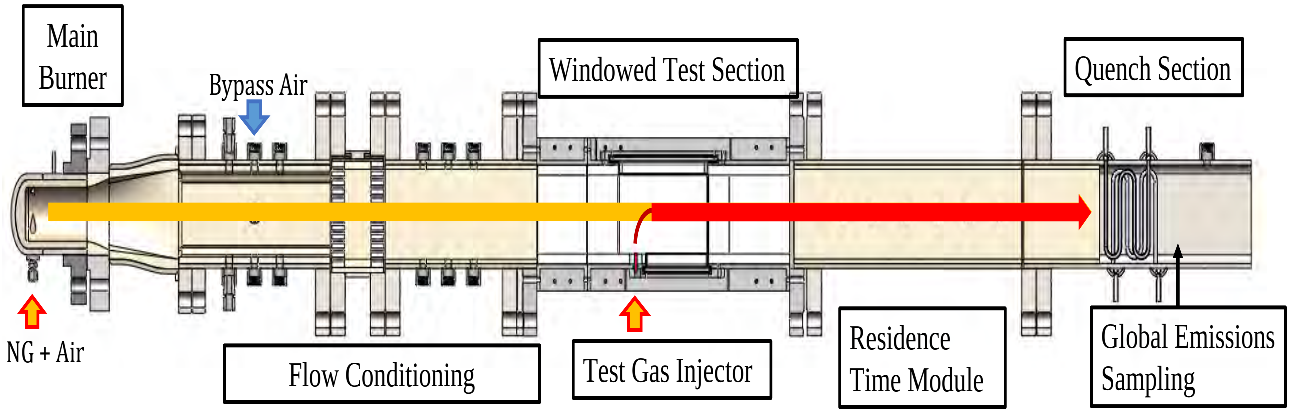
Schematics of re-shocked RMI

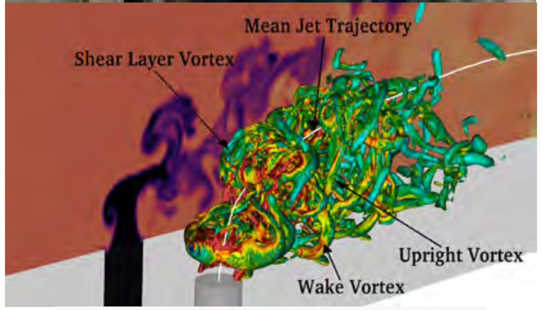


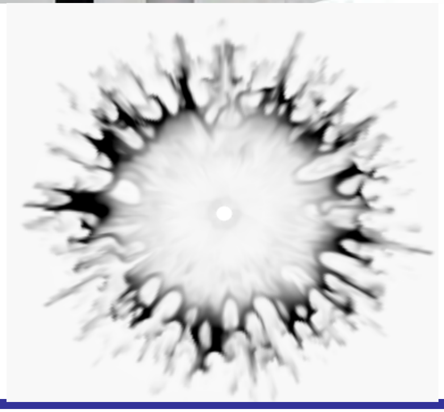




Experimental and Computational Strategies (in RA2-FA3)

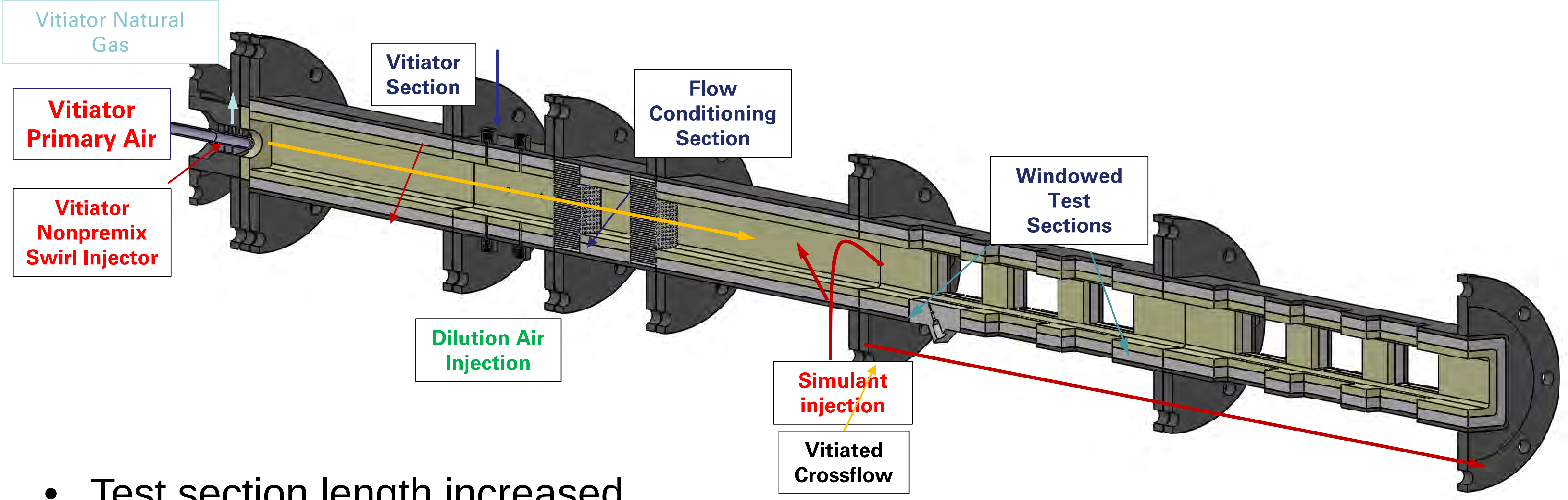






- Experimental facility exists but needs to redesigned
  - Very long run time feasible (> 30 minutes)
  - Test section for diagnostics (PIV, PLIF, GC, etc.) to characterize inflow and mixing
  - JICF with vary injection to mimic mixing time
- Simulation code with UQ capability already exists
  - Code (LESLIE) operational in many DOD labs
  - Leverage capabilities being added for ONR, NASA

Facility Modifications Underway for RA2-FA3

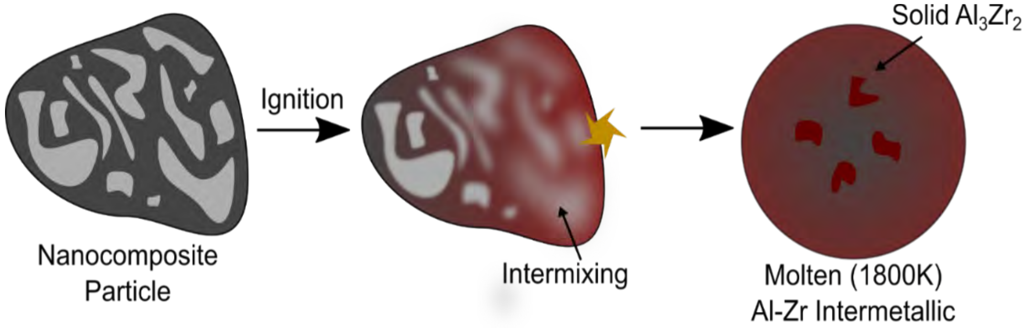


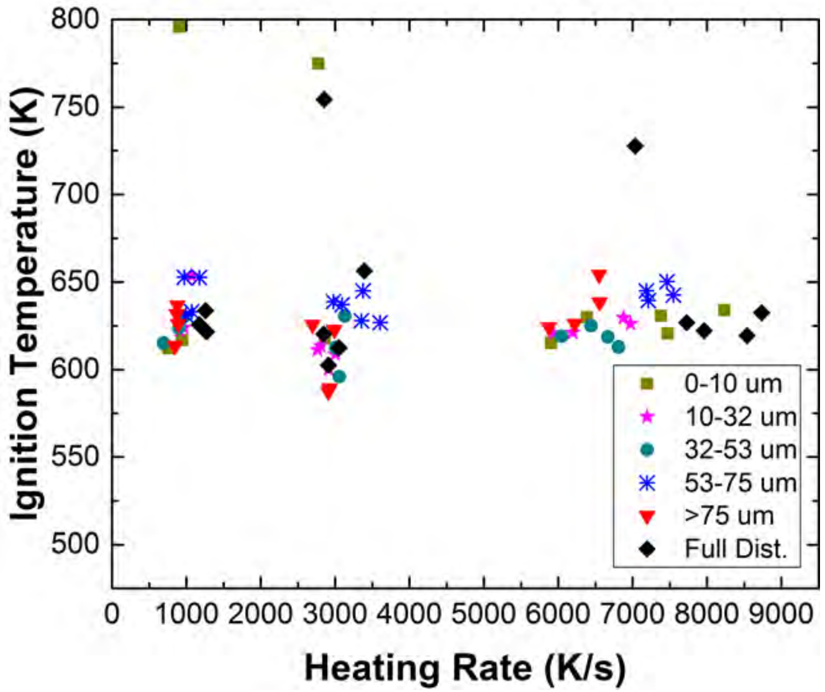
- Test section length increased
- Windows changeable
- Controlled angle injection system
- More diagnostics sensors for inflow

- Design for 1400-1900K vitiated air flow
- Residence time ~ 10-100 ms

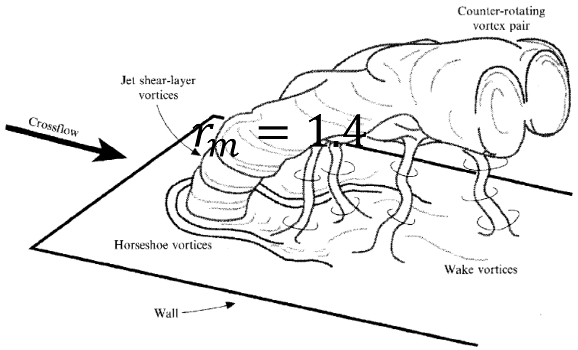
Metal Oxides & Simulant Combustion: RA2-FA3

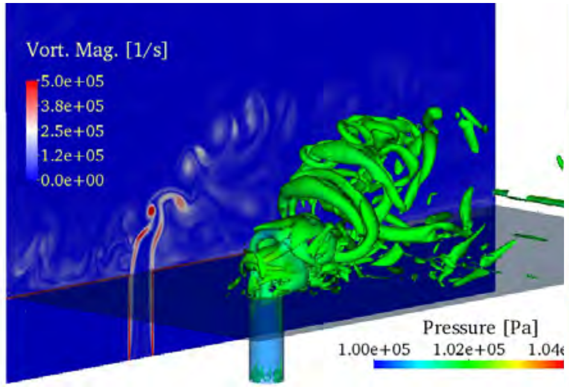
- Leverage work in JHU (T. Weihs)
- Metal particles mixed with simulant
- Mixing and ignition modeling
- Inputs (JHU): kinetics, ignition temperature and time scale to be used in CFD model
- Micro-scale physics needs to be upscaled to macro-scale for large scale simulation: homogenization
- Data from experiments to be used

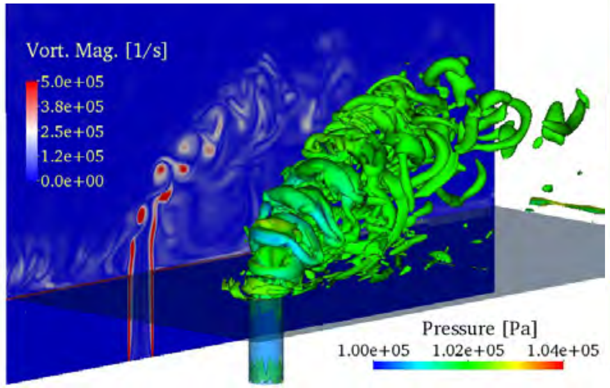


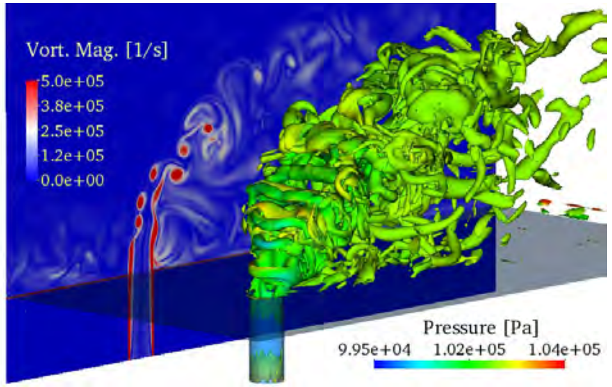


Reacting JICF with Different Momentum Ratio (Past studies)

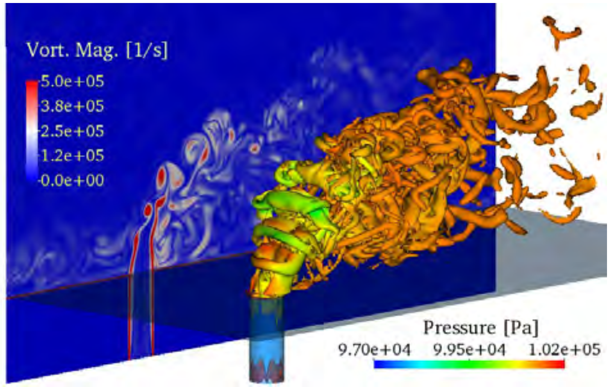




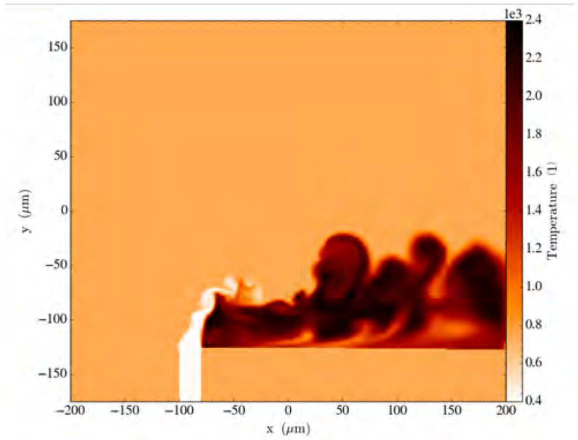


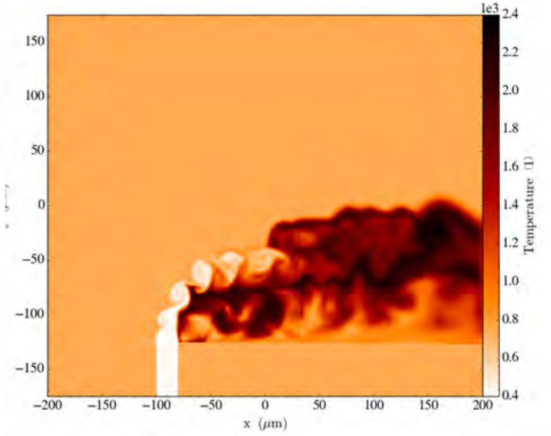


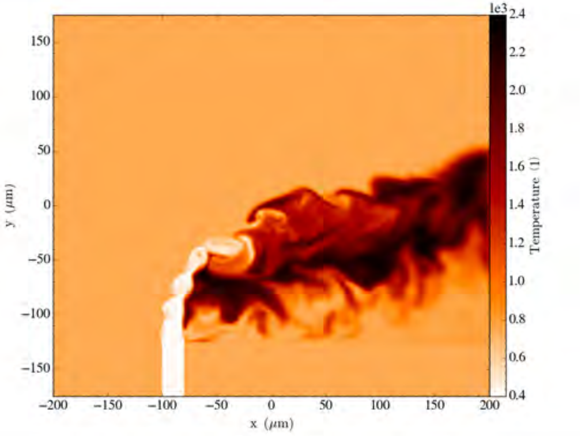
$r_m = 1.4$ $r_m = 2.2$ $r_m = 2.9$



$r_m = 2.2$, nonreacting

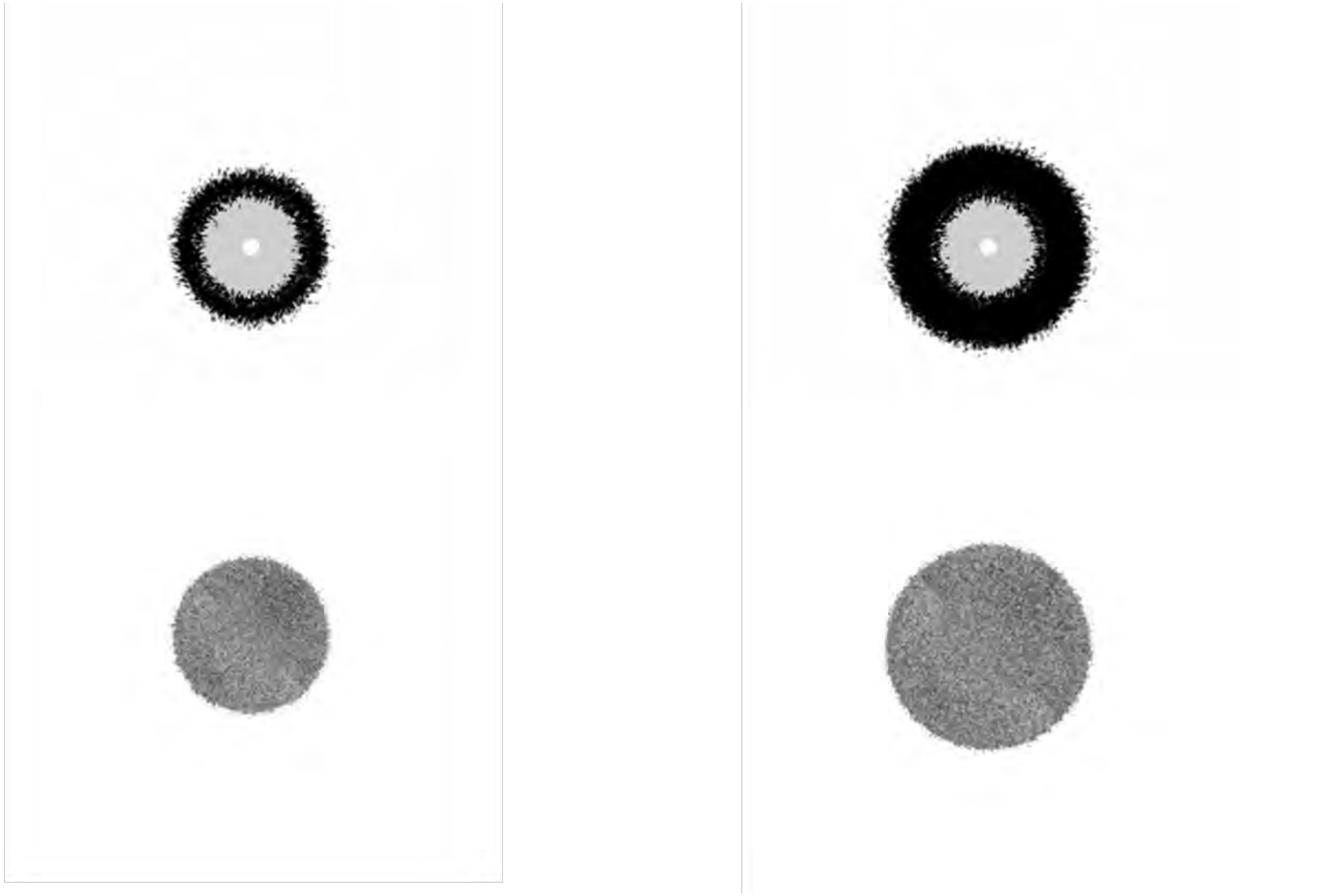






3D Explosion and Afterburning (future application: RA2-FA3)

Bubbles and spikes on
Fireball without particles



Detonation with particles at the interface

What is Revolutionary and/or Unique About this Research

- Fundamental assessment of turbulence-chemistry interactions using relatively realistic CA under relatively realistic conditions
- Parametric variation to capture the range of conditions
- Modeling tools validated against canonical data
- Inputs to models accounts for new discoveries and UQ from other studies under MSEE

Description of PI Activities

- Co-PI (S. Menon, GIT) will direct experimental & numerical effort
  - Collaborate with other researchers in RA3-FA2 and RA2-FA1/FA2 to include latest discoveries in kinetics, UQ modeling and metal oxides
  - Evaluate computationally efficient reduced kinetics for simulants
  - Inverse UQ using surrogate model to assess kinetics
  - LES studies experimental studies in GT
- Co-PI (J. Seitzman, GIT) will lead the diagnostics campaign
  - Measurements for code validation
  - JICF studies as a function of operating parameter
- Co-PI (T. Weihs, JHU) will supply composite powders for combustion studies & provide inputs for oxide modeling

Plans for Collaborative Exchanges

- Planned collaboration with all members in RA3-FA2
- Collaboration with JHU on UQ (CCRI: M. Shields)
- Planned Collaboration with ARL on general EOS modeling
- Both experimental & modeled data will be made available