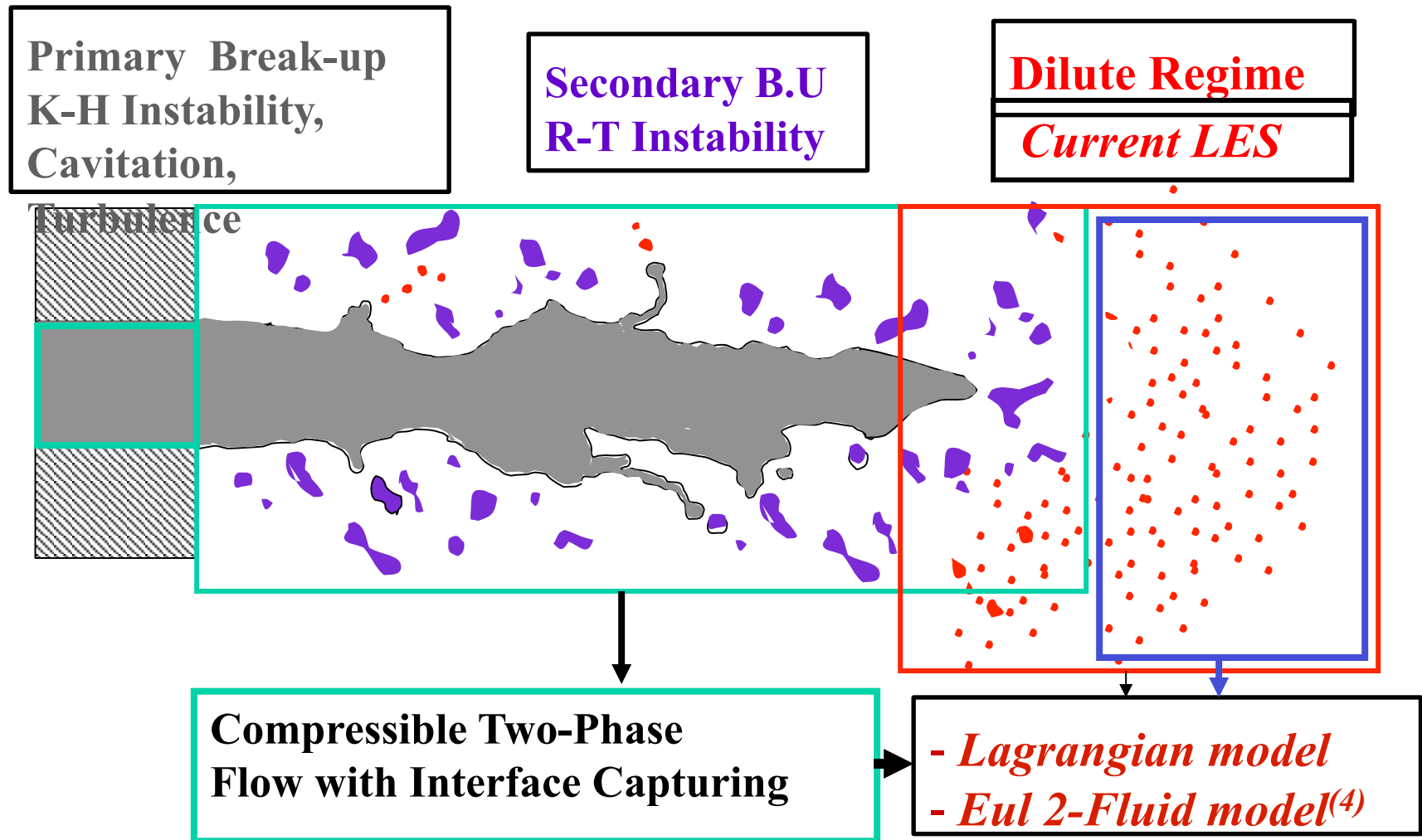


Lecture 7

CFD of Spray Combustion in Gas Turbines

- Spray formulation and implementation issues
- Dump combustors with swirl
 - Operational and laboratory combustors
- Complex geometry, Multiple injectors coupling
- Different numerical strategies by different groups
- Different models by same and/or different groups
- Acknowledgements
 - Thierry Poinsot, IMF Toulouse, CNRS, France
 - Peter Flohr, ALSTOM, Switzerland
 - Joe Oefelein, Sandia National Laboratory, CA

AIAA CFD for Combustion Modeling



Suresh Menon, Georgia Tech

Spray Modeling Strategies

- Eulerian two-fluid approach (e.g. AVBP)
 - Volume fraction is known but droplet size distribution is not explicitly available
 - More cost effective
- Lagrangian droplet tracking approach (e.g., SNL, GT)
 - Each particle or “parcel” is tracked in the Eulerian gas phase with two-way coupling
 - Droplet size distribution can be prescribed
 - Drag laws for different size particles can be included
 - More expensive but perhaps more accurate

Dilute Spray: Modelling Assumptions

- Spherical droplet
 - Droplets deform due to motion
 - Drag correlations are based on spheres of equivalent volume, which “takes” this effect into account.
- Dilute approximation
 - Valid if $v_f/v_g < 0.001$.
 - Not usually valid in the near field of injectors where a breakup model becomes necessary.
 - Drag correlations can be justified under this approximation
 - Particle collision effects are neglected
- Pressure at drop location is constant
- Coriolis, Basset, Gravity forces etc. are ignored.
 - $\rho_l / \rho_g \gg 1$

Dilute Sprays: Modelling Assumptions

- Droplet radius smaller than Kolmogorov scale
 - Interaction between droplet and gas is dominated by laminar fluid dynamics
 - Heat conduction can be ignored if $Bi < 0.1$
 - Radiation between drop and surroundings is neglected
- Oxidation process neglected in the flow field around drop
 - Droplet Damkohler number too small for envelope flames, wake flames, etc.

Gas Phase Equations

- Liquid-gas phase coupling through source terms.

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_i}{\partial x_i} = \dot{\bar{\rho}}_s$$

$$\frac{\partial \bar{\rho} \tilde{u}_i}{\partial t} + \frac{\partial}{\partial x_j} [\bar{\rho} \tilde{u}_i \tilde{u}_j + \bar{p} \delta_{ij} - \bar{\tau}_{ij} + \tau_{ij}^{sgs}] = \dot{\bar{F}}_{s,i}$$

$$\frac{\partial \bar{\rho} \tilde{E}}{\partial t} + \frac{\partial}{\partial x_i} [(\bar{\rho} \tilde{E} + \bar{p}) \tilde{u}_i + \bar{q}_i - \tilde{u}_j \bar{\tau}_{ji} + H_i^{sgs} + \sigma_i^{sgs}] = \dot{\bar{Q}}_s$$

$$\frac{\partial \bar{\rho} \tilde{Y}_k}{\partial t} + \frac{\partial}{\partial x_i} [\bar{\rho} \tilde{Y}_k \tilde{u}_i - \bar{\rho} \tilde{Y}_k \tilde{V}_{i,k} + Y_{i,k}^{sgs} + \theta_{i,k}^{sgs}] = \dot{\bar{w}}_k + \dot{\bar{S}}_{s,k} \quad k = 1, N_s$$

$$\begin{pmatrix} \dot{\bar{\rho}}_s \\ \dot{\bar{F}}_{s,i} \\ \dot{\bar{Q}}_s \\ \dot{\bar{S}}_{s,k} \end{pmatrix} = - \begin{pmatrix} \frac{dm_d}{dt} \\ \frac{dm_d u_i}{dt} \\ \frac{dm_d e_d}{dt} \\ \frac{dm_d Y_m}{dt} \end{pmatrix} = - \begin{pmatrix} \rho_d \frac{dV_d}{dt} + V_d \frac{d\rho_d}{dt} \\ m_d \frac{du_{i,d}}{dt} + u_{i,d} \frac{dm_d}{dt} \\ m_d \frac{de_d}{dt} + e_d \frac{dm_d}{dt} \\ m_d \frac{dY_{m,d}}{dt} + Y_{m,d} \frac{dm_d}{dt} \end{pmatrix}$$

Filtered Conservation Equations

- Mass:

$$\frac{\partial}{\partial t}(\theta \bar{\rho}) + \nabla \cdot (\theta \bar{\rho} \tilde{\mathbf{u}}) = \bar{\rho}_s$$

- Momentum:

$$\frac{\partial}{\partial t}(\theta \bar{\rho} \tilde{\mathbf{u}}) + \nabla \cdot \left[\theta \left(\bar{\rho} \tilde{\mathbf{u}} \otimes \tilde{\mathbf{u}} + \frac{\mathcal{P}}{M^2} \mathbf{I} \right) \right] = \nabla \cdot (\theta \bar{\vec{\tau}}) + \bar{\mathbf{F}}_s$$

- Total Energy:

$$\frac{\partial}{\partial t}(\theta \bar{\rho} \tilde{e}_t) + \nabla \cdot [\theta (\bar{\rho} \tilde{e}_t + \mathcal{P}) \tilde{\mathbf{u}}] = \nabla \cdot \left[\theta \left(\bar{\vec{Q}}_e + M^2 (\bar{\vec{\tau}} \cdot \tilde{\mathbf{u}}) \right) \right] + \theta \bar{\vec{Q}}_e + \bar{\vec{Q}}_s$$

- Species:

$$\frac{\partial}{\partial t}(\theta \bar{\rho} \tilde{Y}_i) + \nabla \cdot (\theta \bar{\rho} \tilde{Y}_i \tilde{\mathbf{u}}) = \nabla \cdot (\theta \bar{\vec{S}}_i) + \theta \bar{\dot{\omega}}_i + \bar{\dot{\omega}}_{s_i}$$

Oefelein, J. C. (2006). Large eddy simulation of turbulent combustion processes in propulsion and power systems. *Progress in Aerospace Sciences*, 42: 2-37.

Subgrid-Scale Model for Particle Dispersion

$$\dot{\bar{\mathbf{F}}}_s(\mathbf{x}, t) = \underbrace{\int_{-\infty}^t \sum_p \mathcal{G}(\mathbf{y}_p - \mathbf{x}, \tau - t)}_{(ii)} \underbrace{\left\{ m_p \frac{d\mathbf{u}_p}{d\tau} \right\}}_{(i)} d\tau$$

(iii)

- **Instantaneous** particle motion tracked in Lagrangian frame as succession of SGS eddies traversed

- **Decompositions of the form**
 $\mathbf{u}_p(\mathbf{x}, t) = \mathbf{U}_p(\mathbf{x}, t) + \mathbf{u}_p''(\mathbf{x}, t)$
reconstructed
- **Fluctuations generated stochastically assuming isotropic and Gaussian**
- **Stochastic intervals coincident with particle-eddy interaction time**

- **Particles interact with eddies for time taken as smaller of eddy lifetime or transit time**

- (i) Instantaneous force induced by particles at remote points \mathbf{y}_p and times τ
- (ii) Spatially filtered effect of remote exchange processes on discrete points \mathbf{x} within filter volume of influence
- (iii) Filtered effect of sgs temporal disturbances over the integration time-step $\delta\tau$

Two-way coupling by evaluating individual contributions imposed by each particle

Explicit filtering of the particulate phase is performed using a top-hat filter

Oefelein, J. C. (2006). Large eddy simulation of turbulent combustion processes in propulsion and power systems. *Progress in Aerospace Sciences*, 42: 2-37.

Mass Conservation

$$\frac{dm_d}{dt} = -\dot{m}_d$$

$$\frac{\dot{m}_d}{\dot{m}_{Re_d=0}} = 1 + [0.278\sqrt{Re_d}Sc^{1/3}] \left[1 + \frac{1.232}{Re_dSc^{4/3}} \right]^{1/2}$$

$$Re_d = \sqrt{(u_i - u_{i,d})(u_i - u_{i,d})}d_d/\nu$$

$$Sc = \nu/D$$

- Experimental data used for most of these correlations
- Effect of turbulence can be considered in the Reynolds number through a fluctuation term computed from KSGS
- However, other than this there is no difference between LES and RANS spray models

Momentum Conservation

$$\frac{dx_{i,d}}{dt} = u_{i,d}$$

$$\frac{du_{i,d}}{dt} = \frac{f}{\tau_V} [(u_i) + u_i'' - u_{i,d}]$$

- Effect of small scales through subgrid KE and a random number factor to compute u''

- Drag factor

$$f = \frac{C_D Re_D}{24}$$

$$C_D = \begin{cases} \frac{24}{Re_d} (1 + \frac{1}{6} Re_d^{2/3}) & Re_d \leq 1000 \\ 0.424 & Re_d > 1000 \end{cases}$$

- Particle response time

$$\tau_V = \frac{\rho_d d_d^2}{18\mu_g}$$

Energy Equation

$$m_d C_L \frac{dT_d}{dt} = h_d \pi d_d^2 (\tilde{T} - T_d) - \dot{m}_d L_v \quad (16)$$

- L_v is the latent heat of vaporization, h_d is the heat transfer coefficient

$$\frac{h_d}{h_{Re_d=0}} = 1 + 0.278 Re_d^{1/2} Pr^{1/3} / \left[1 + \frac{1.232}{Re_d Pr^{4/3}} \right]^{1/2}$$

$$h_{Re_d=0} = \frac{\kappa Nu_{Re_d=0}}{d_d} \quad Nu_{Re_d=0} = 2 \ln \left(\frac{\alpha}{\alpha - 1} \right)$$

Droplet Time Scales

- Modelling physics at the appropriate timescales necessary to accurately capture the transient dynamics of droplet combustion.
- Droplet relaxation time $\tau_v = \frac{16\rho_d r_d^2 (C_D Re_d)^{-1}}{3\rho_g v}$
 - Time required for droplet to reach 63% of the free stream velocity
- Droplet lifetime $\tau_{life} = \frac{4\pi r_d^3 \rho_d}{3\dot{m}_d}$
 - Ensure that droplet size does not become negative within a Lagrangian time step
- Droplet Heating time scale $\tau_{evap} = \frac{\rho_d C_v d_d}{6h_d}$
 - Ensures that local mass loading does not create numerical instability

Droplet Time Scales

- Eddy life and transit time
 - Drop interacts with the eddy for its life time or the time required to traverse the eddy.

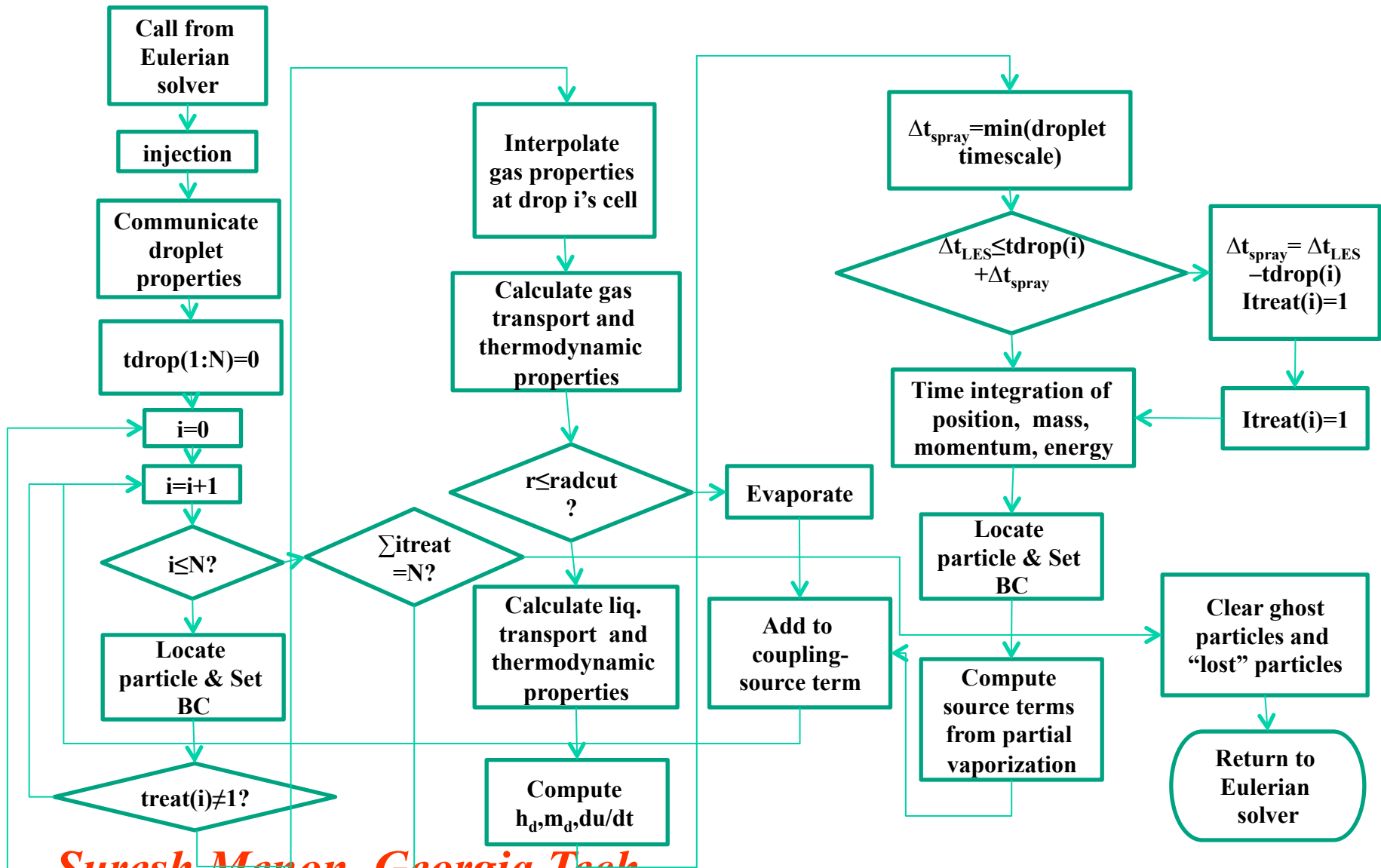
$$\tau_{eddy} = \Delta / \sqrt{(2k^{sgs}/3)}$$

$$\tau_{transit} = \tau_{relax} \ln\left(1 - \frac{\Delta}{(\tau_{relax}|u_i - u_{i,d}|)}\right)$$

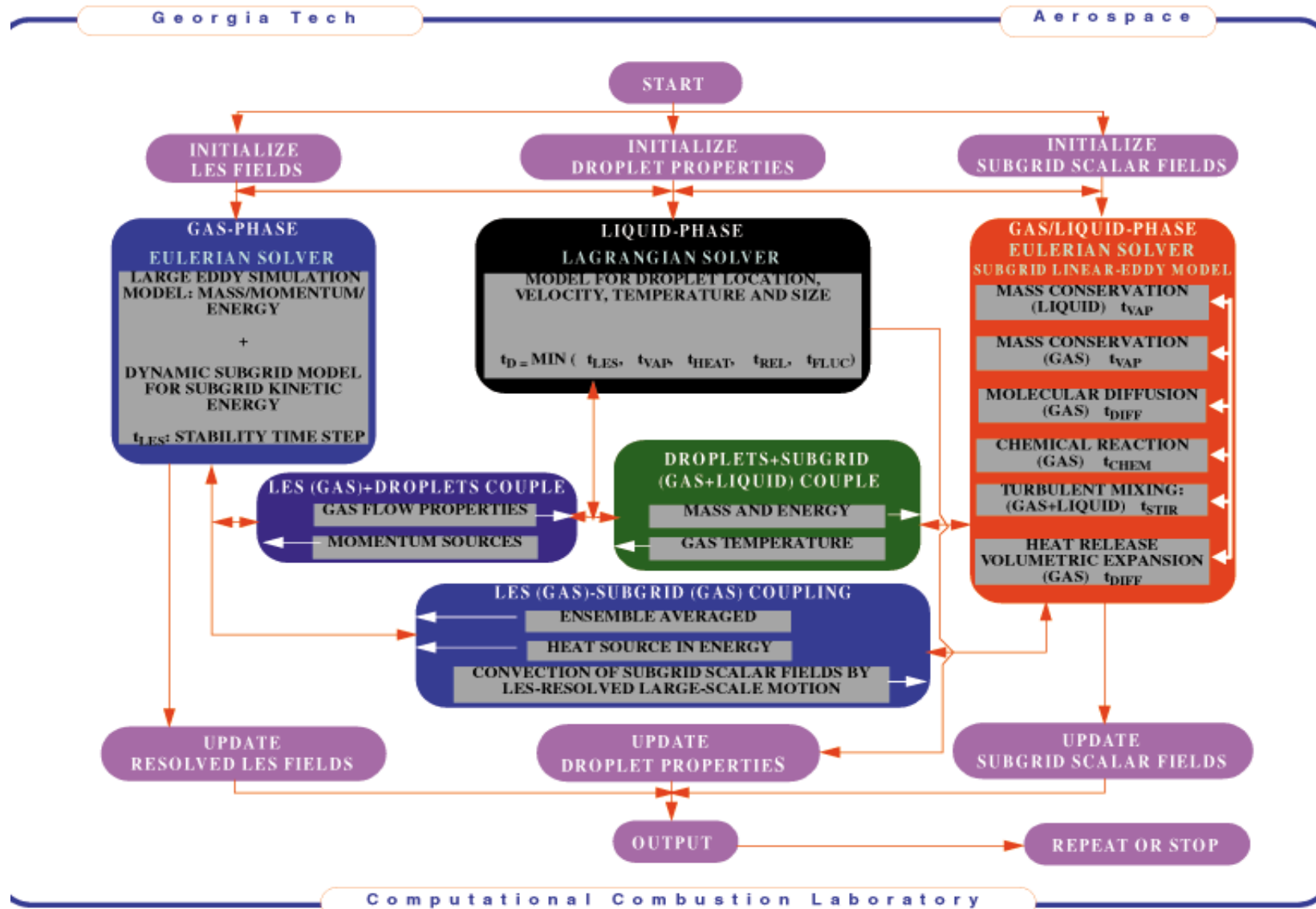
$$\tau_{eddy \text{ int}} = \begin{cases} \tau_{eddy} & , \Delta > \tau_{relax}|u_i - u_{i,d}| \\ \min(\tau_{eddy}, \tau_{transit}), & \Delta \leq \tau_{relax}|u_i - u_{i,d}| \end{cases}$$

$$\Delta t = \min(\tau_{evap}, \tau_{life}, \tau_{relax}, \tau_{eddy}, \tau_{transit}, \tau_{LES})$$

Algorithm



AIAA CFD for Combustion Modeling



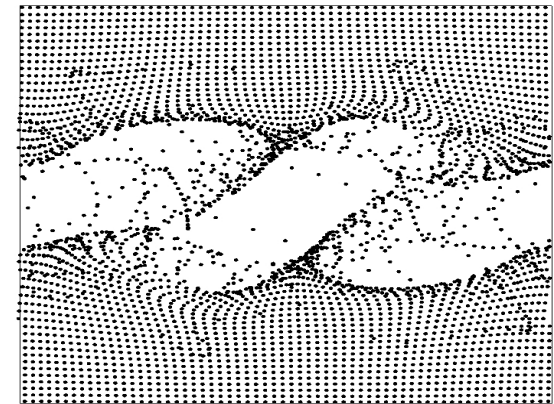
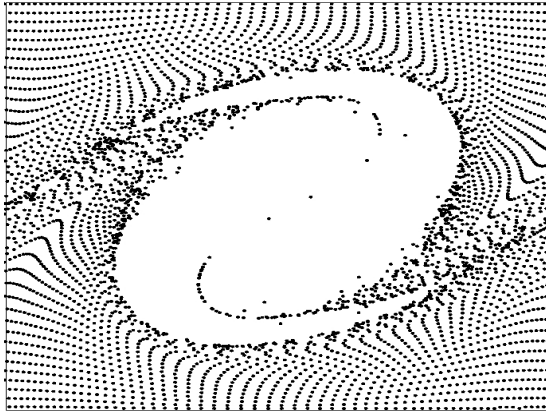
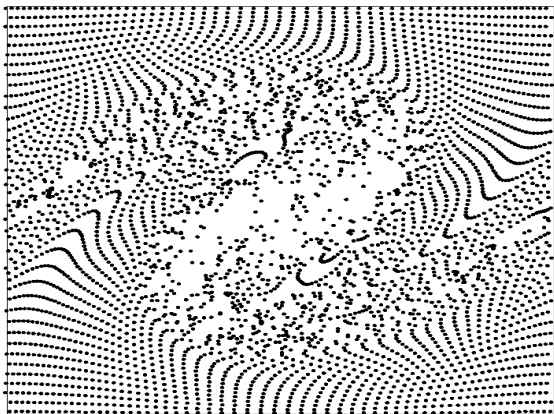
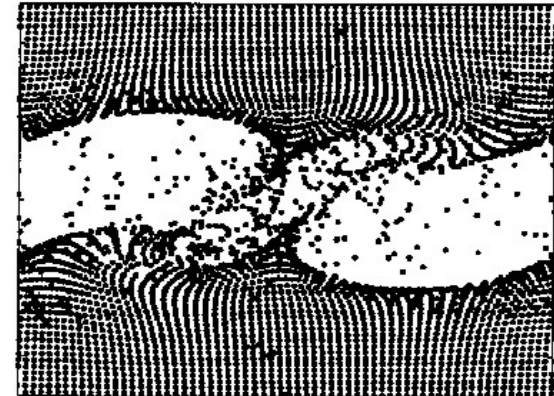
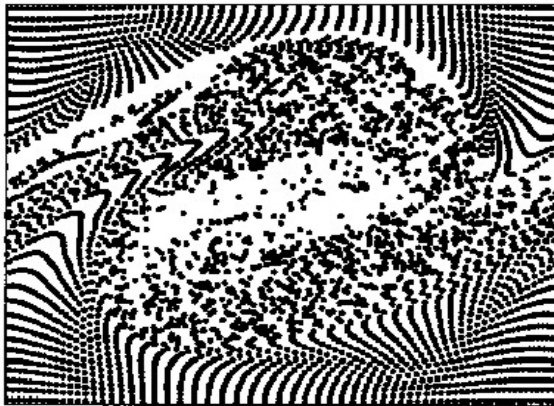
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Implementation and Modeling Issues

- Injector exit flow field (spray distribution, velocities etc) has to be defined for dilute spray modeling
- For breakup – models are needed
 - Still not fully resolved
 - All current models are based on RANS studies
 - K-H instability, TAB model, etc.
- Parallel implementation
 - Gather-scatter
 - Point-to-point
 - Advantages and disadvantages of each approach

DNS of Particle Laden Mixing Layers

Top row: Ling et al., JFM 98, Bottom row: Menon, 2005

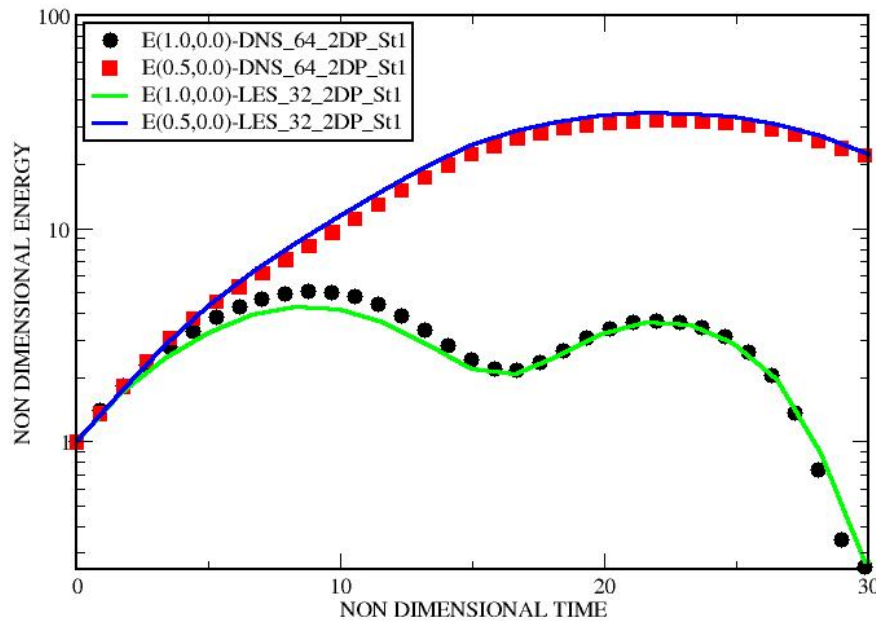


St = 0.1

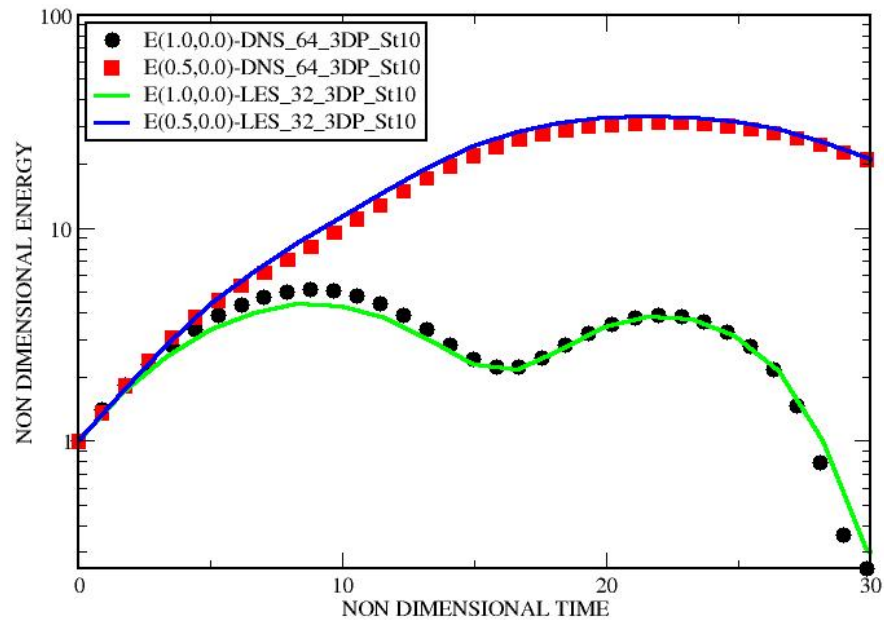
St = 1

St = 100

Comparison of LES and DNS in Particle Laden Temporal Mixing Layer



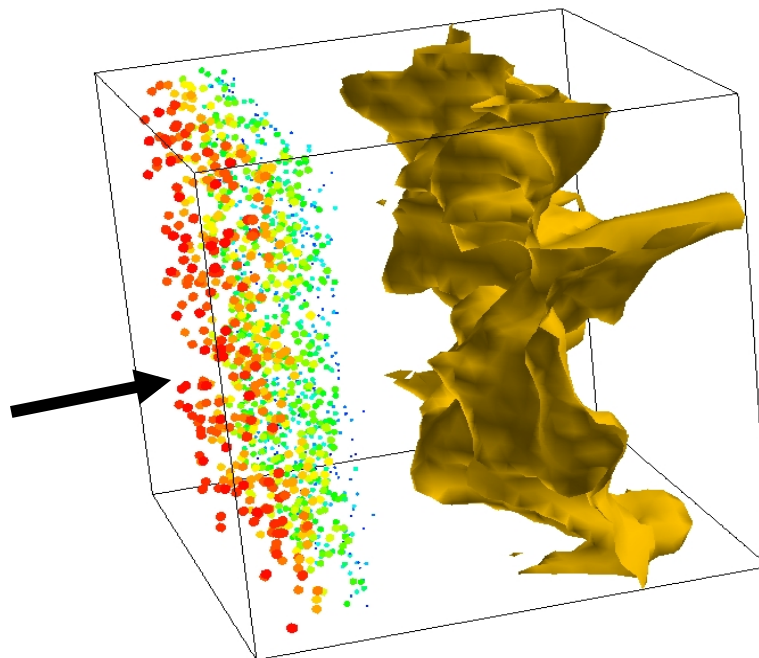
St =1



St =10

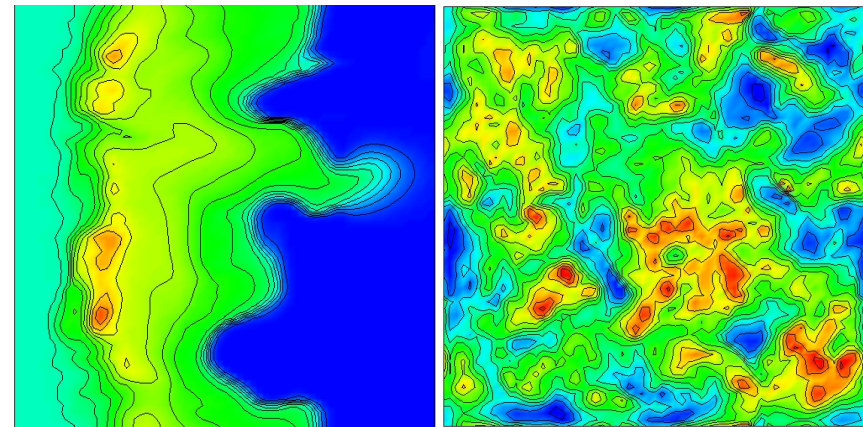
DNS: 643, O(4), LES: 32**3, O(4), Dynamic k-sgs model
2 Mode Initialization: Fundamental and Subharmonic**

LES of Partially Premixed Combustion in Two-Phase Mixtures



X-Y Plane

Y-Z Plane

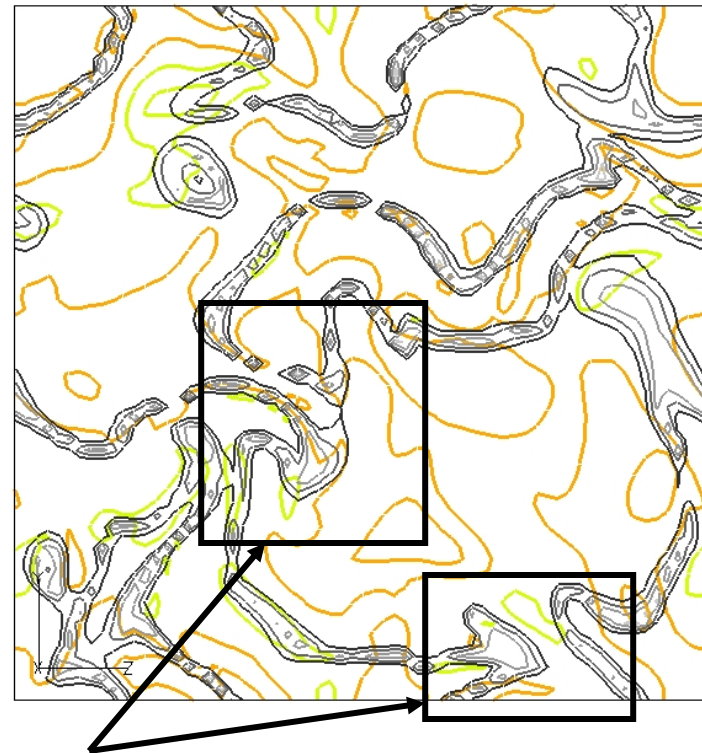
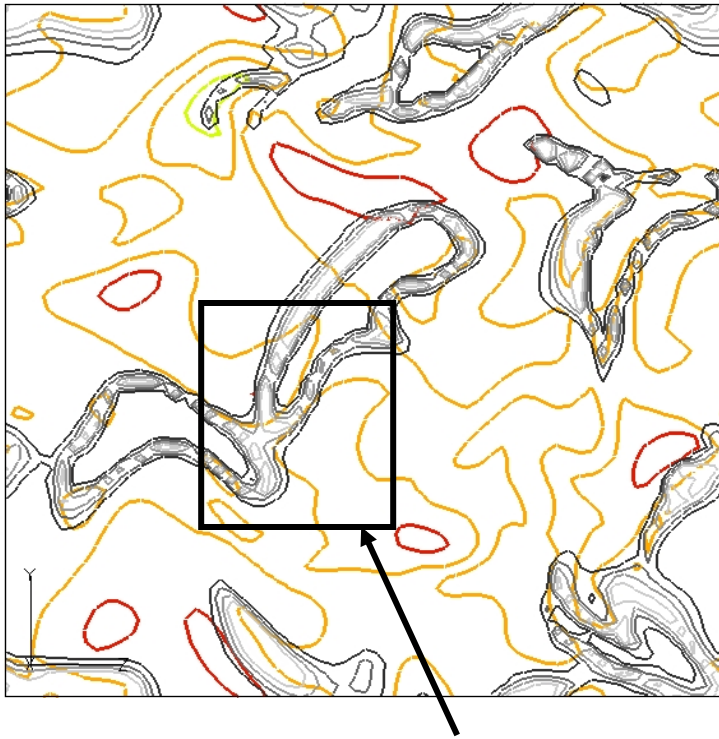


Contours of Methane Mass Fraction just before the flame

Lean Methane-air Premixed Mixture with 5-10 (blue-red) micron Methanol droplets, Overall Equivalence Ratio of 0.8. Grid is 643 with 18 LEM cells per LES cell.**

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Fine-Scale Flame Structure in Partially Premixed Two-Phase Mixture



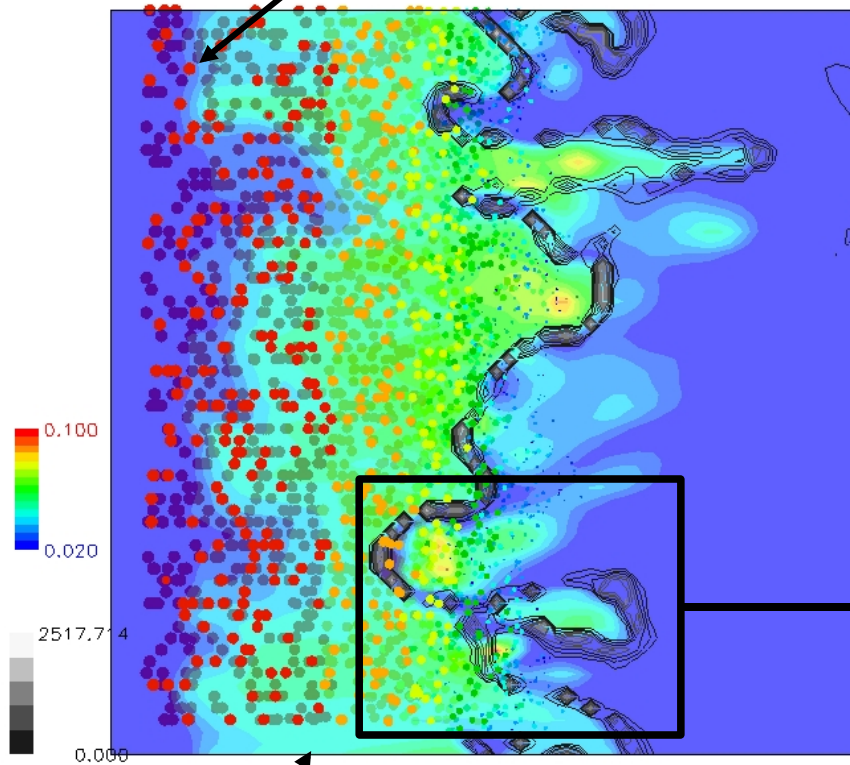
Triple-Flame Structure in the Flame Zone

Contours of Reaction Rate (BLACK) and Mixture Fraction (COLOR)

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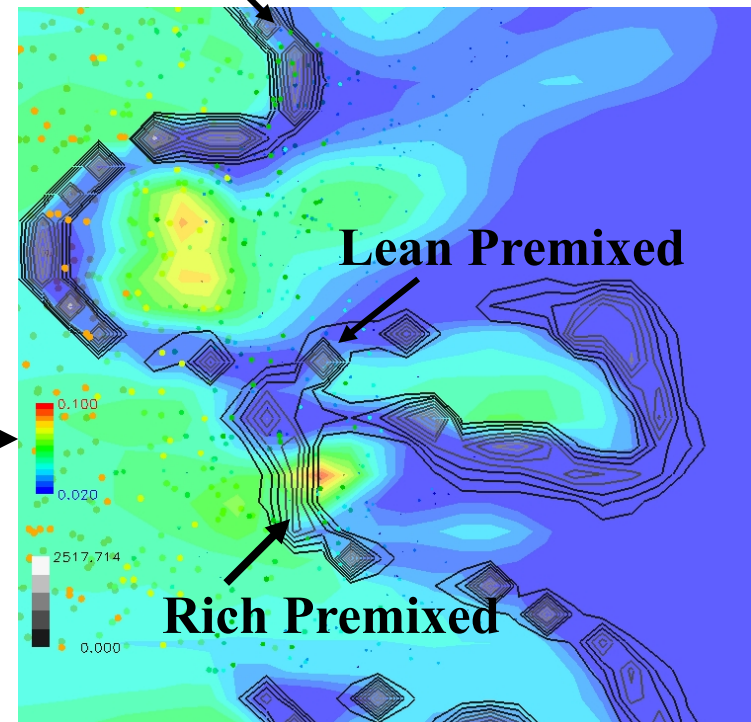
Triple-Flame Structure in Two-Phase Flame Zone

Methanol Droplets (Log Normal, SMD= 40)

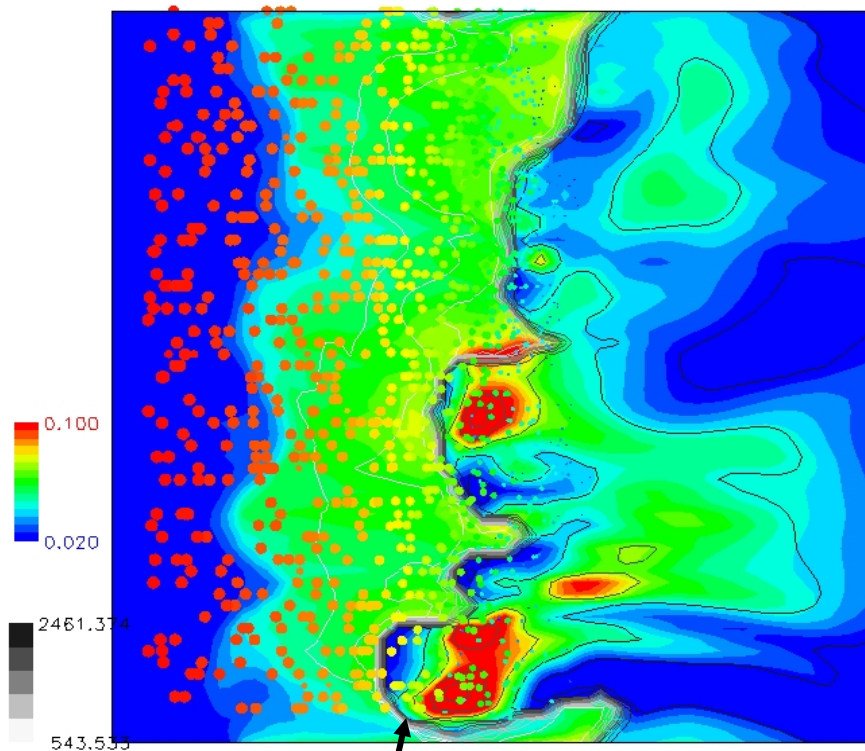


Methane Fuel Vapor (LES Filtered)

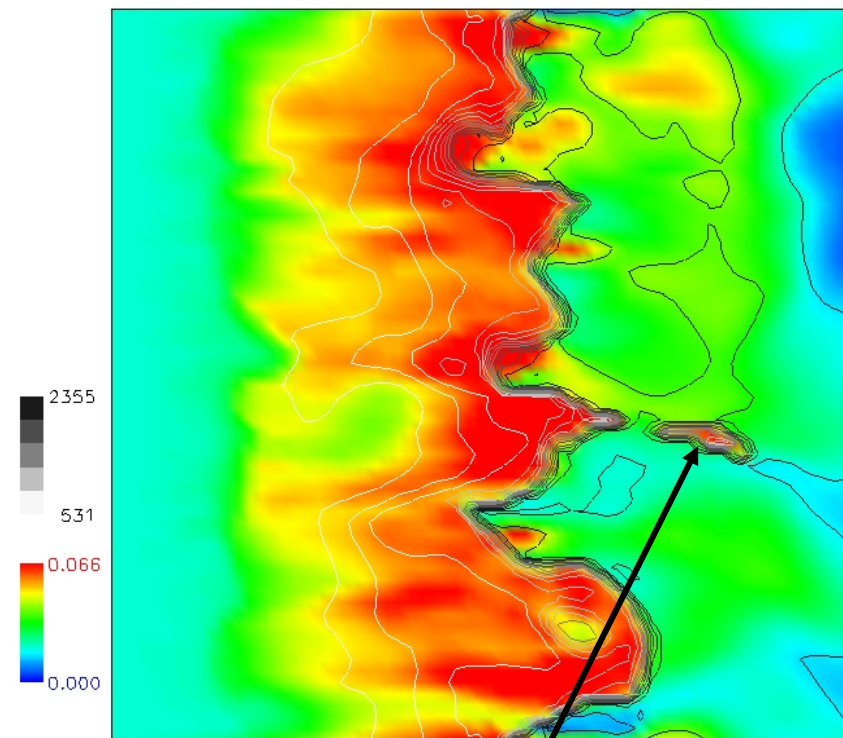
Reaction Rate (LES Filtered)



Flame Structure around Droplets



Connected Flame around Droplet Clusters



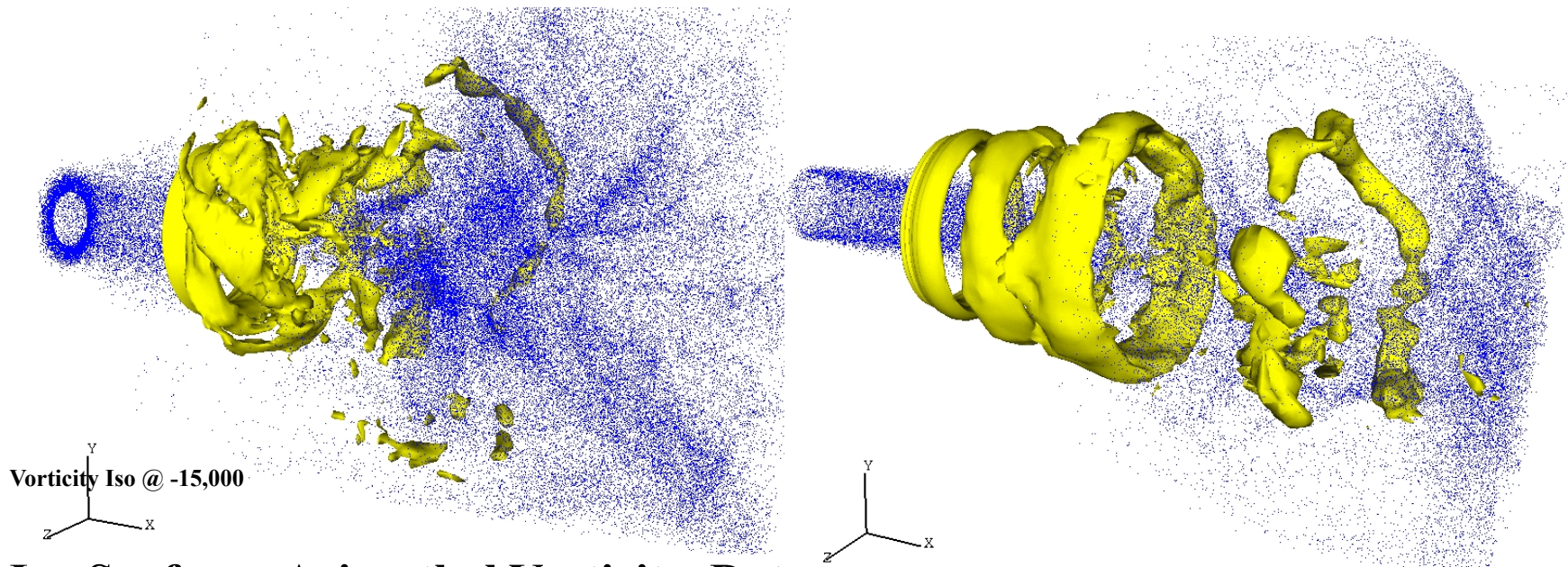
Disconnected Flame around Droplet Clusters

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Effect of Swirl on Spray Dispersion in a General Electric DACRS Gas Turbine Combustor

Non-Reacting HIGH Swirl

Non-Reacting LOW Swirl

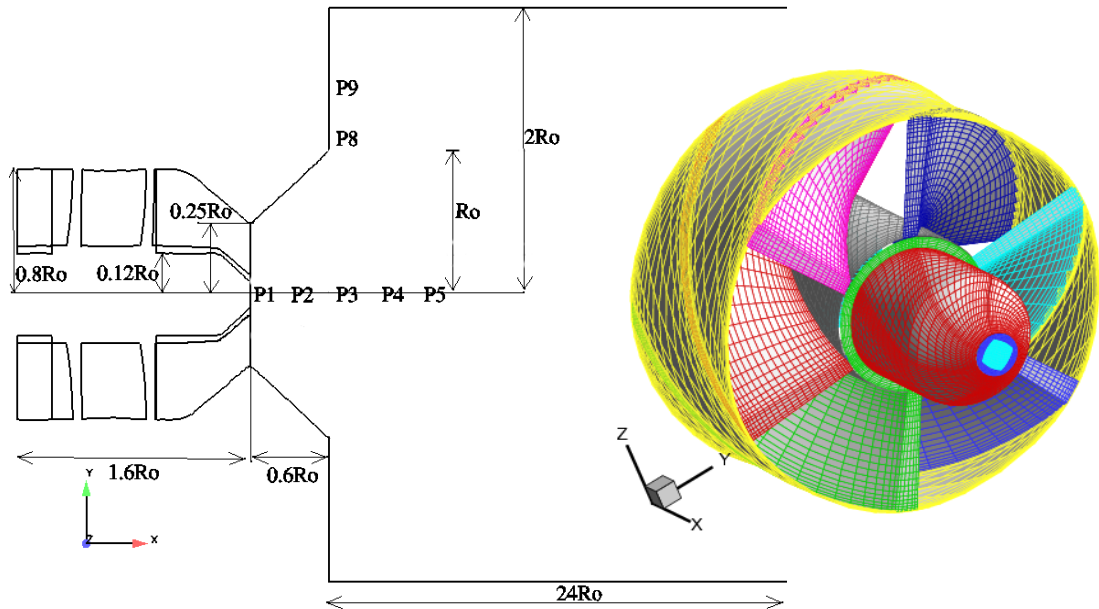
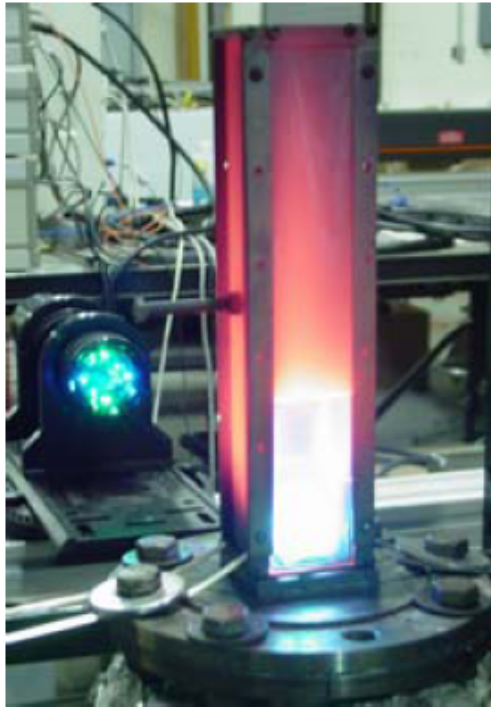


Iso-Surface : Azimuthal Vorticity, Dots: Droplets (40 micron).

Vortical structures in low swirl flow are more coherent and they modulate droplets motion resulting in lower dispersion, mixing and hence, inefficient combustion.

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LDI Experimental Setup



Experimental Setup; Cai *et al.*

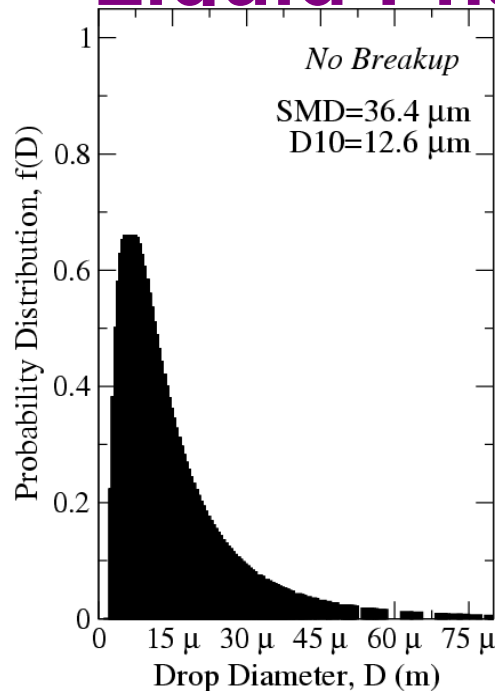
Computational Domain

- Assembly consists of six 60° helical swirl vaned inlet
- Ensuing Swirl number is 1.0; $R_o=12.6$ mm; $U_{BULK}=20$ m/s
- Butterfly domain of 1.5 M nodes; $y^+ \sim 6$ swirler vane walls

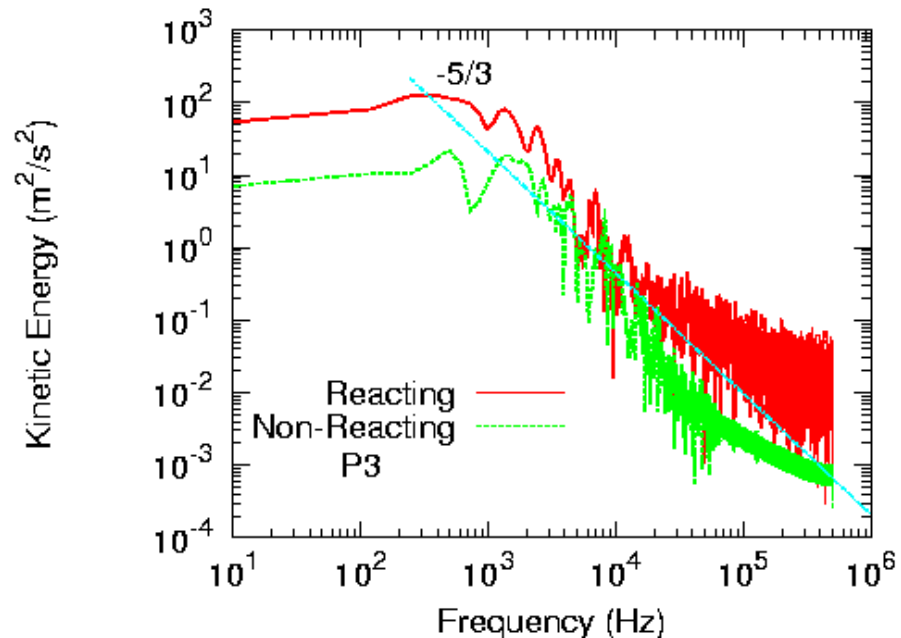
Gas-Phase Inflow Conditions

- **Through-The-Vane (TTV) simulation performed**
 - **Eliminates need to prescribe inflow velocity profiles**
 - **Turbulence generation ensues from flow through vanes**
- **Measurements performed at:**
 - **Atmospheric pressure, 300 K air, Overall $\varphi \sim 0.75$**
 - **Experimental Jet-A fuel approx as $C_{12}H_{23}$**
 - **$Re_D \sim 30,759$ (based on bulk flow & inlet diameter)**
 - **$Re_\Delta \sim 56$ (based on κ^{sgs} & LES filter width)**
- **Chemistry:**
 - **3-step, 7-species, Global reduced mechanism**
 - **Arrhenius rates adapted from Westbrook & Dryer for first two steps & Malte *et al.* for NO chemistry**

Liquid-Phase Initial Conditions



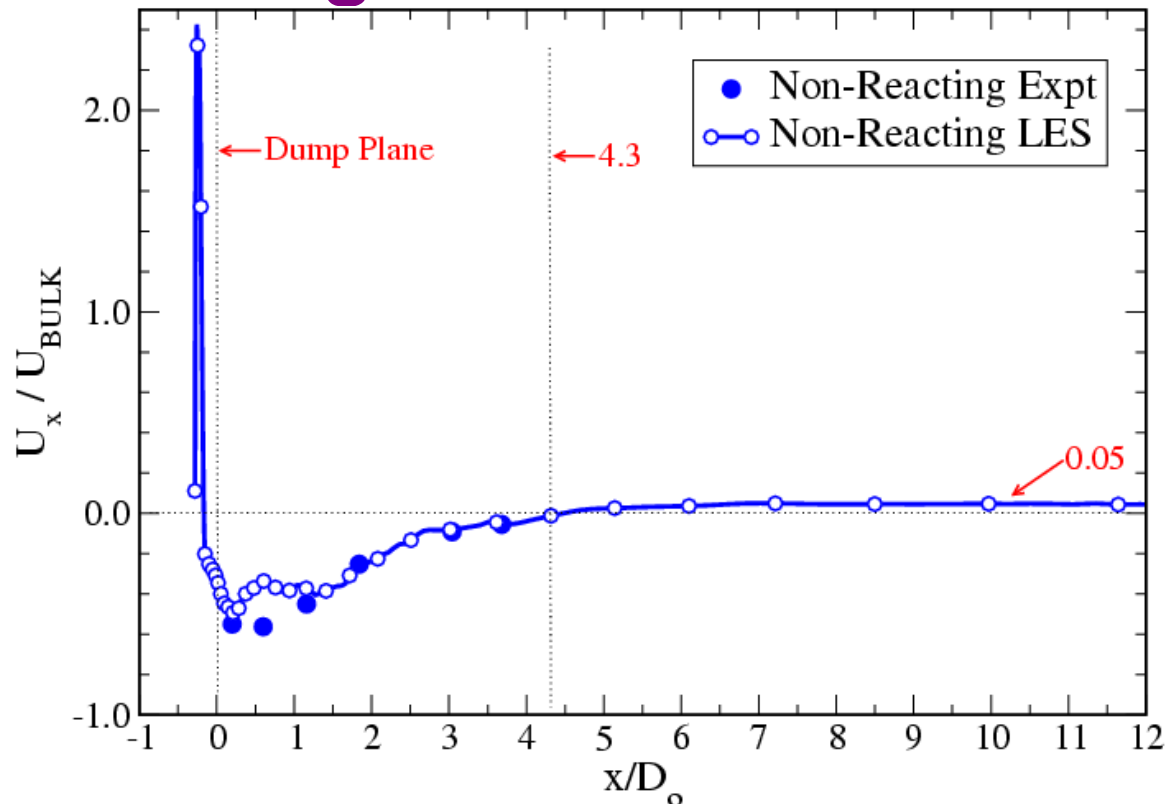
Initial Droplet Distribution



Kinetic Energy Spectra

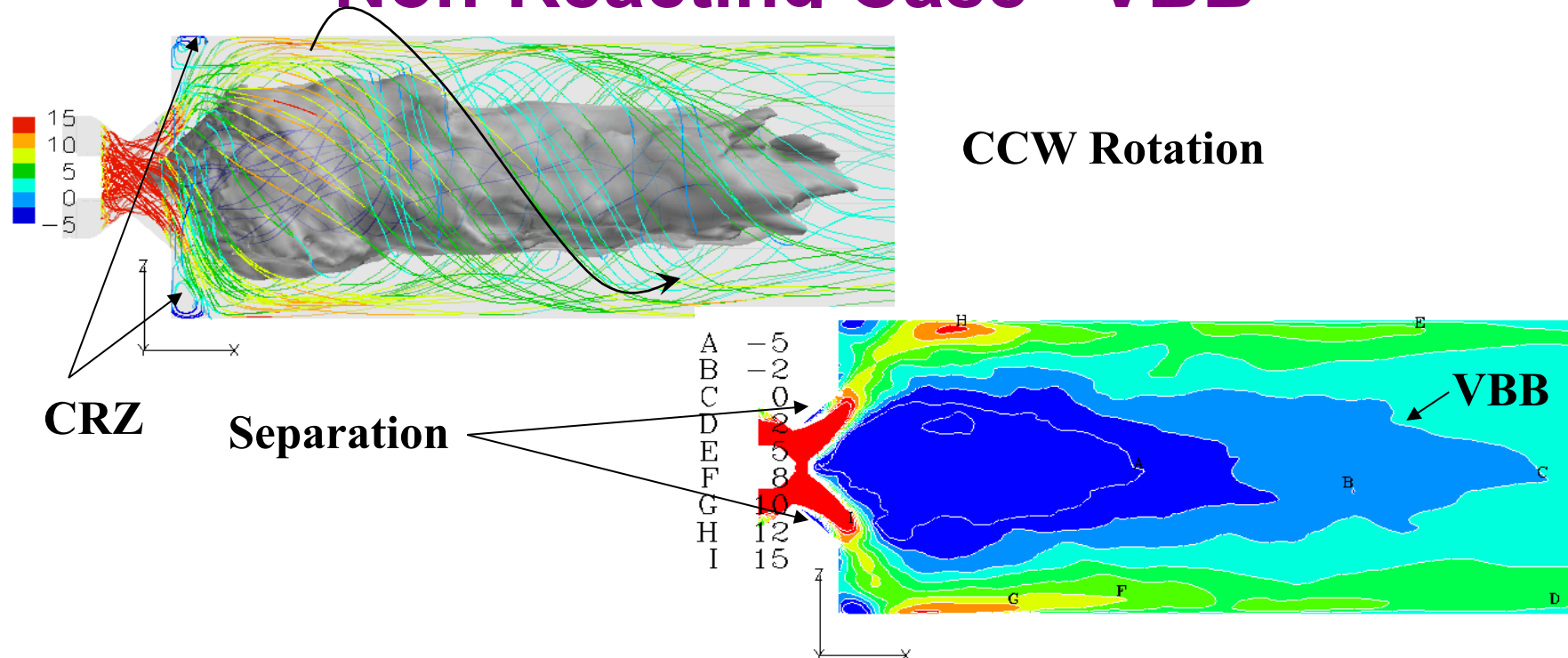
- Log-normal droplet size distribution w/ 36.4 μm SMD
 - Spray data chosen to match near injector data
- Droplet cut-off radius ~ 1 mm; Approx. 25,000 parcels
- Grid resolution is adequate to recover some inertial range for both non-reacting & reacting cases

Non-Reacting Centerline Axial Velocity



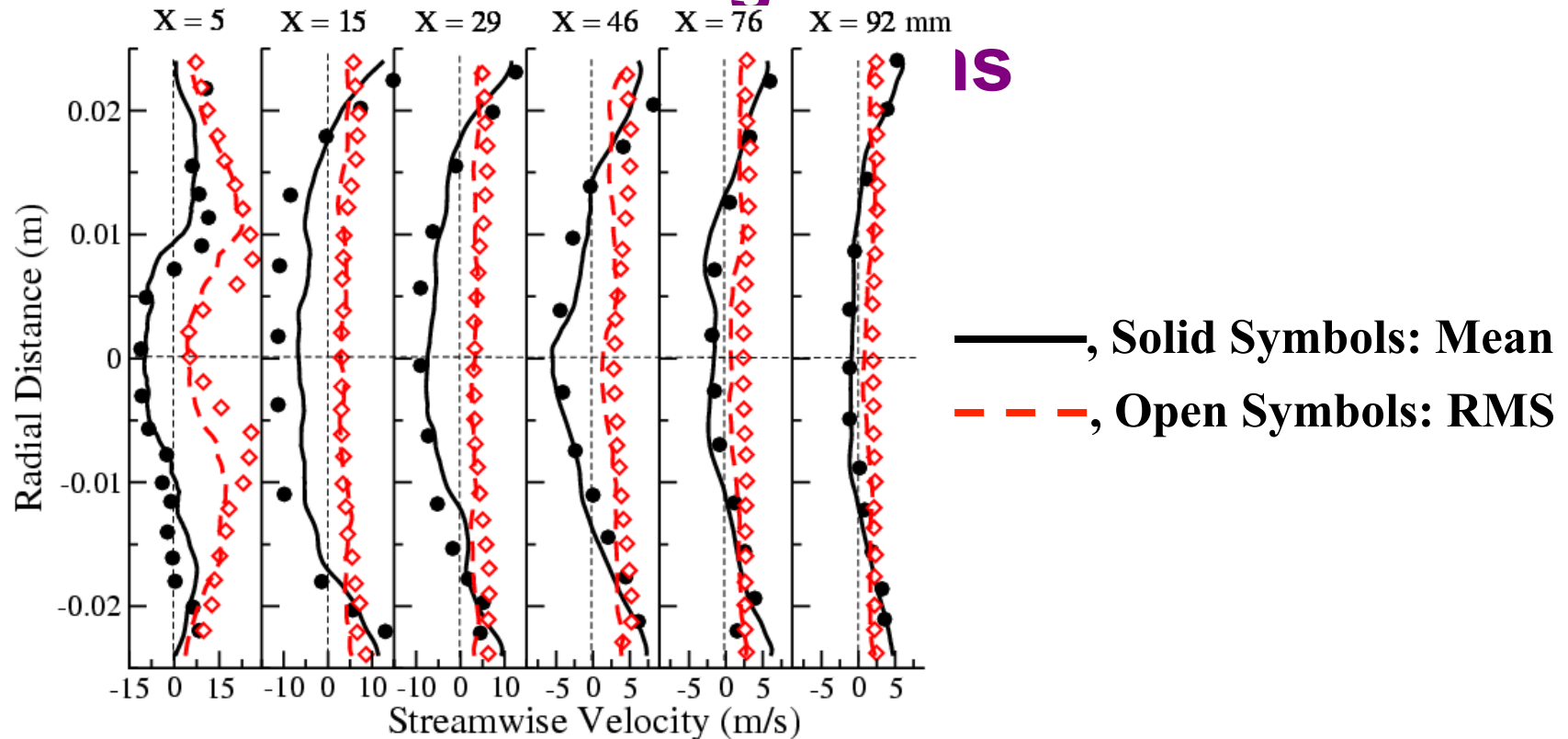
- VBB length $x/D_0 \sim 4.3$; Recovery velocity $\sim 5\%$ of U_{BULK}
- Peak negative $\sim 60\%$; Peak Positive $\sim 240\%$ of Bulk
- Strength & Extent of VBB reasonably predicted by LES

Non-Reacting Case - VBB



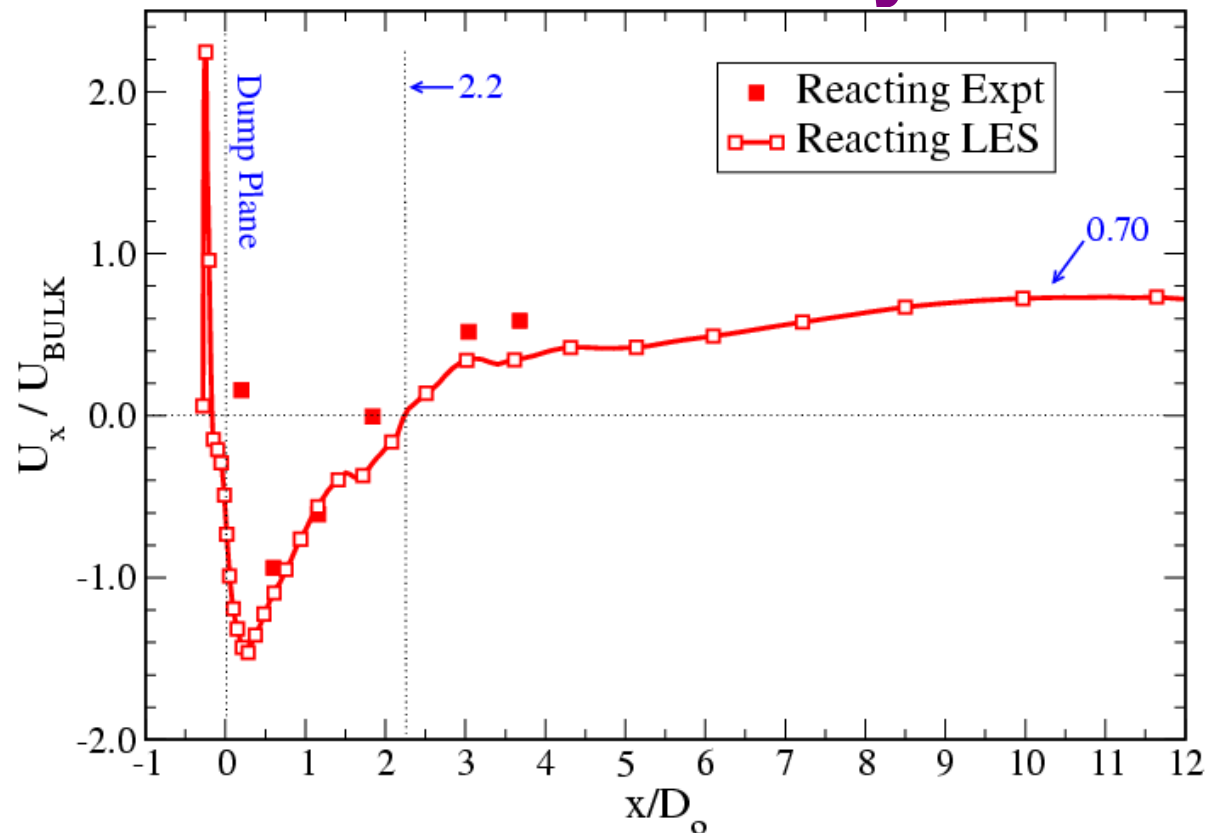
- VBB (iso-surface) is a single contiguous region
- Corner re-circulation zone (CRZ) noted
- Leaf-shaped cross-section for VBB in the center-planes
- Strong TKE observed between VBB and venturi walls

Non-Reacting Case - Axial



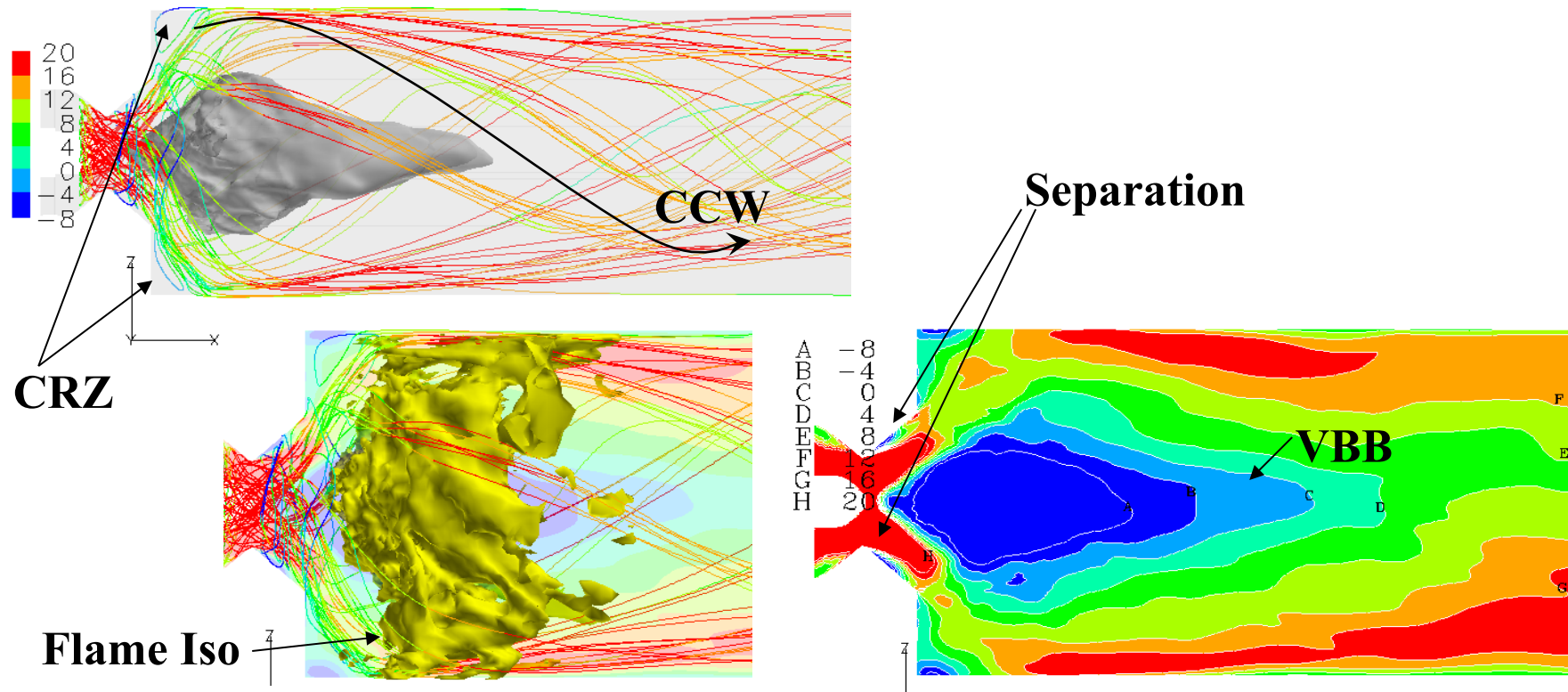
- Radial extent of VBB: $r/R_0 \sim 1.4$ @ $x/R_0 \sim 1.0$
- RMS profile peaks indicates shear-layer regions
- RMS decays and approaches uniform radial profiles

Centerline Axial Velocity - Reacting



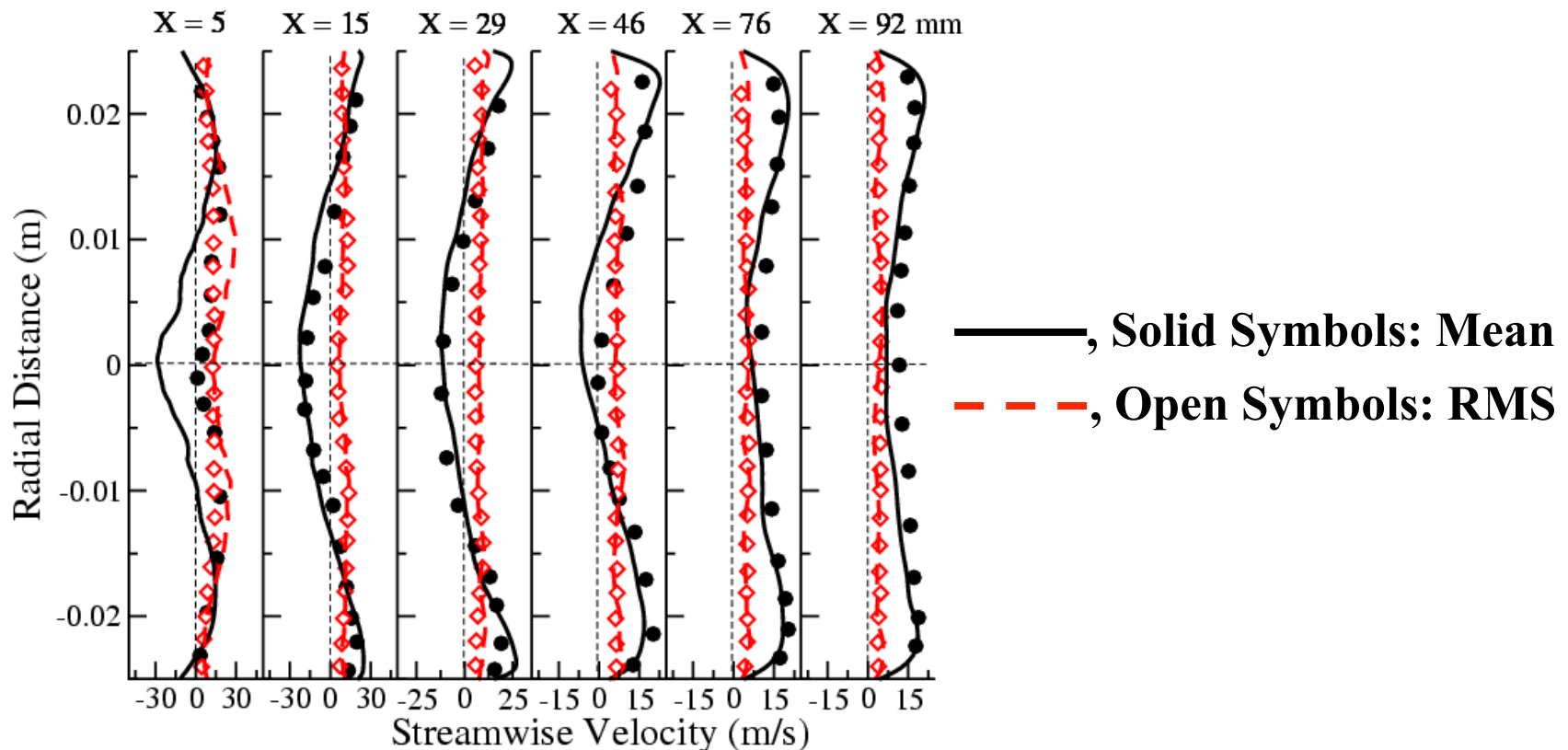
- VBB length $x/D_0 \sim 2.2$; Recovery vel $\sim 70\%$ of U_{BULK}
- Peak negative $\sim 160\%$; Peak Positive $\sim 240\%$ of Bulk
- Strength & Extent of VBB reasonably predicted by LES

Reacting Case - VBB



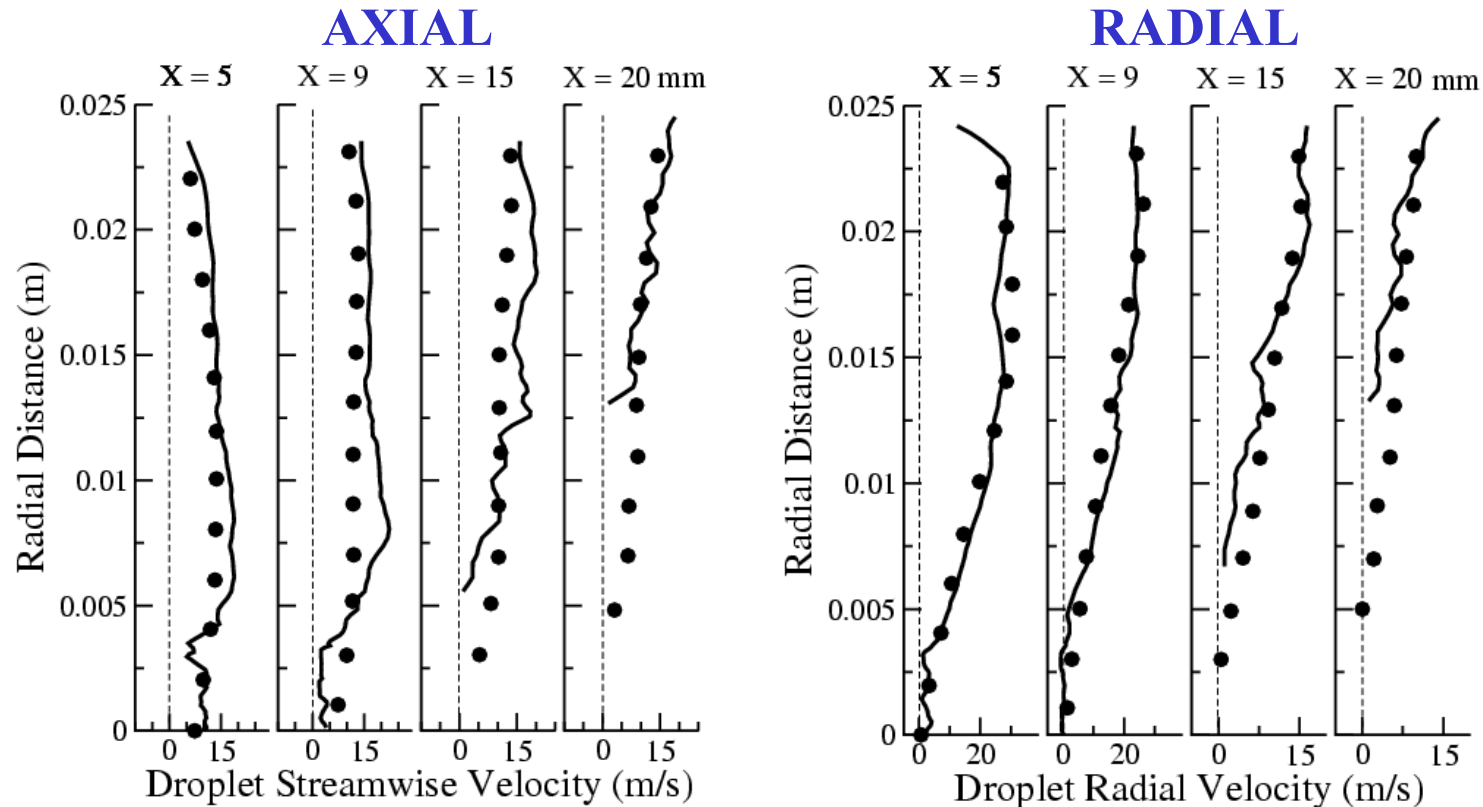
- VBB is a single contiguous region albeit smaller
- Separation seen at 45° expansion angle, CRZ noted as well
- Mean flame surface stabilized by the VBB

Reacting Case - Axial Comparisons



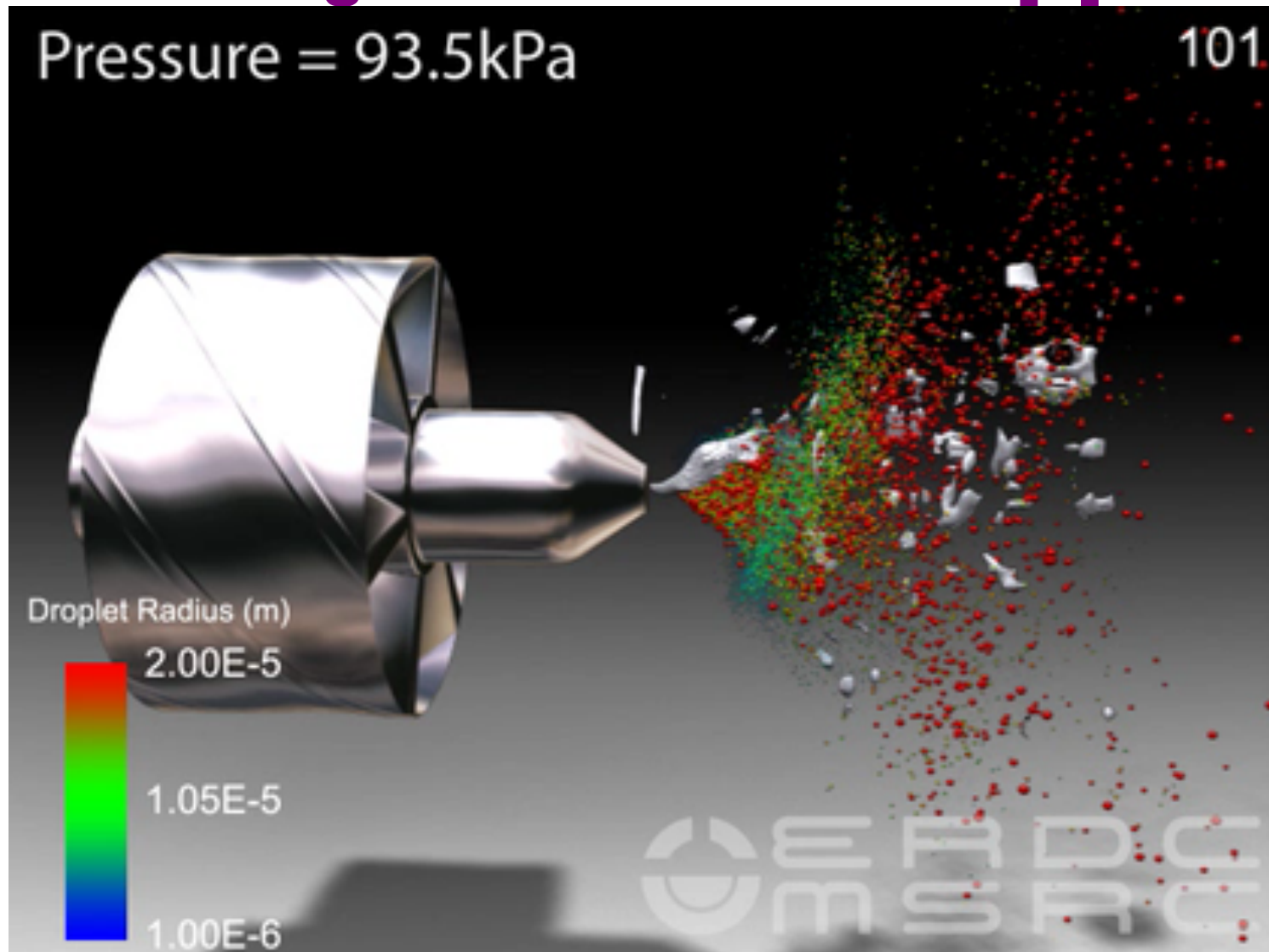
- Radial extent of VBB: $r/R_0 \sim 1.0$ @ $x/R_0 \sim 1.0$
- Peak in axial velocity found on outer edges, Wall-jet effect
- RMS decays, uniform profile downstream; 30% intensity

Reacting - Particle Velocity

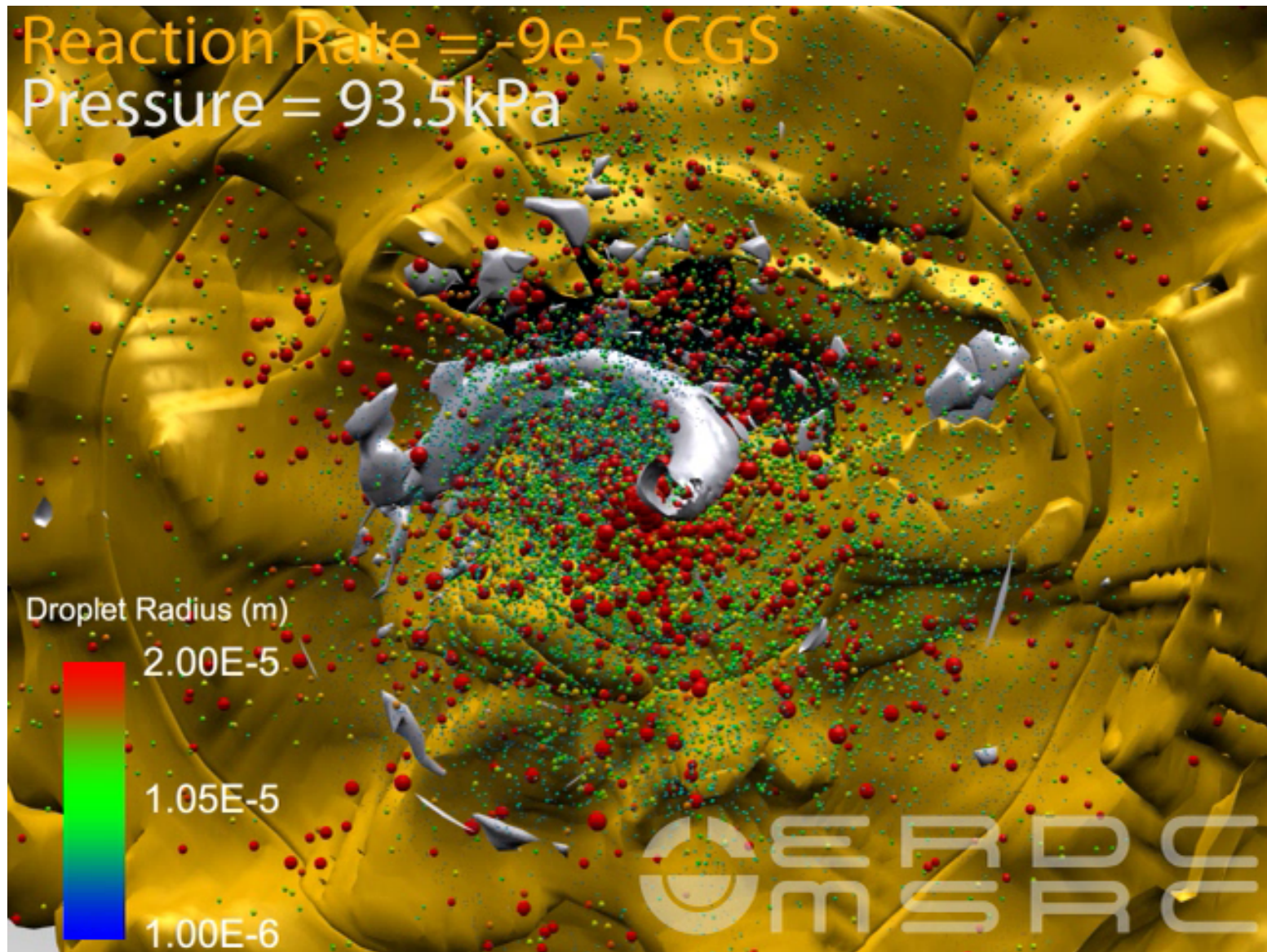


- Particle comparisons for 31-45 μm diameter bin
- Particle path seen to form a hollow-cone shape
- Positive axial velocity observed in VBB; Good trend noted

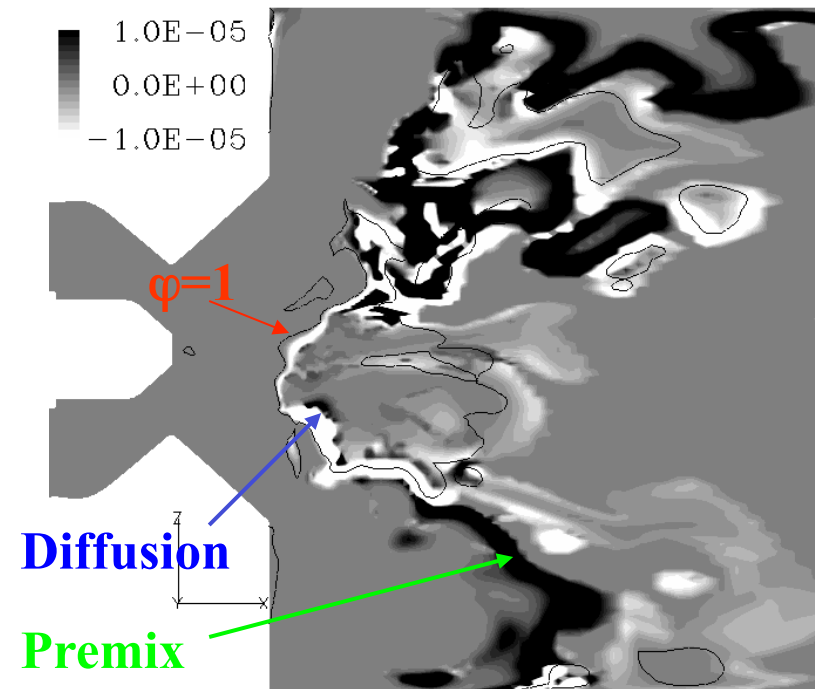
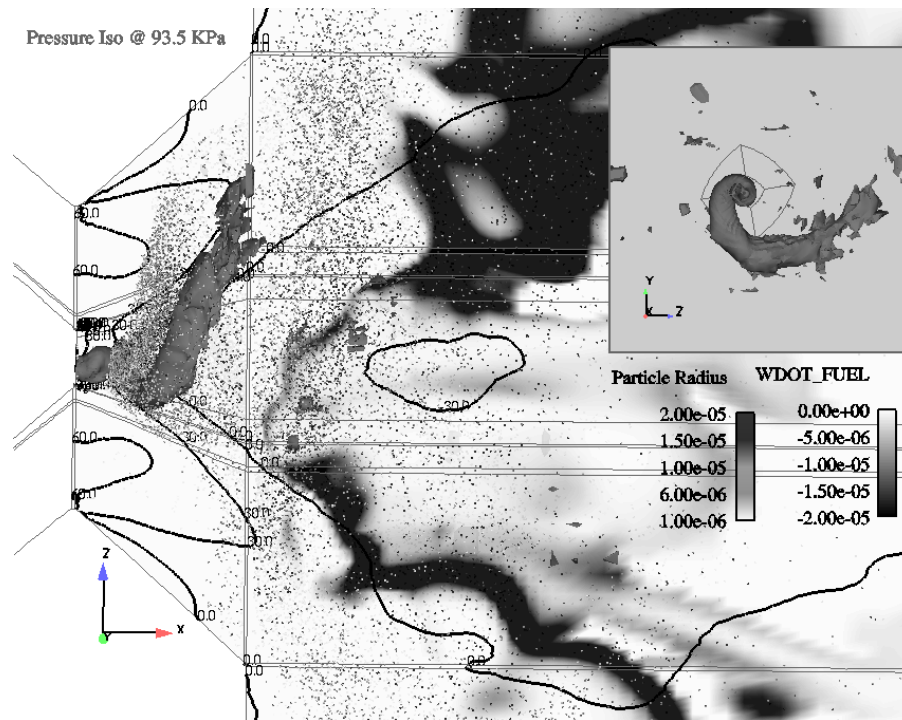
Reacting Case – Animation [1]



Reacting Case – Animation [2]



Reacting Case - Flame Structure

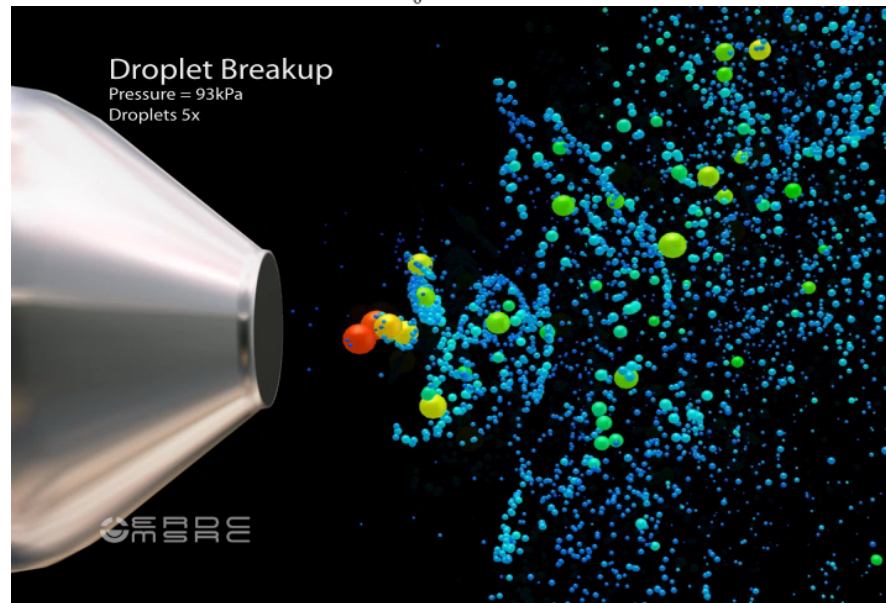
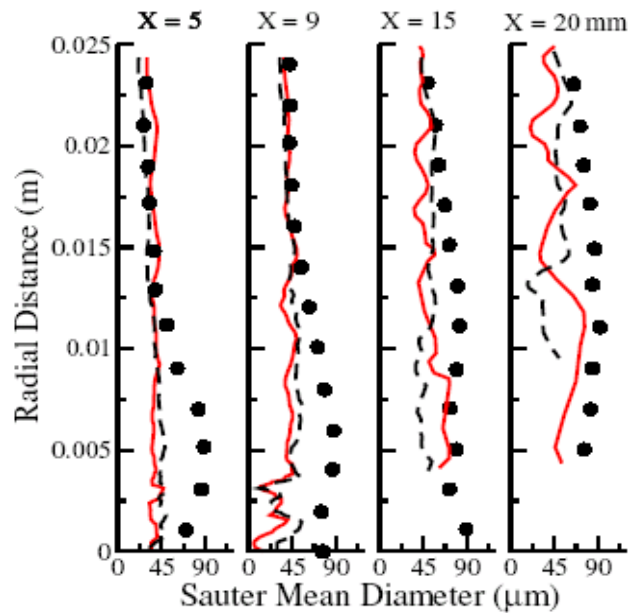
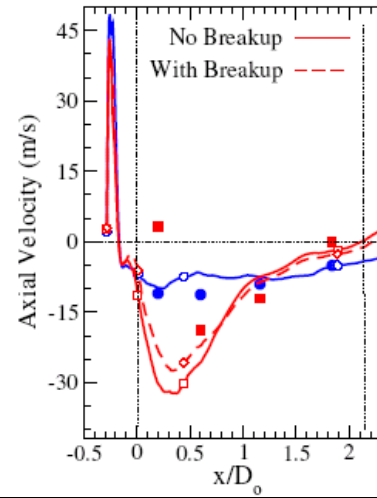
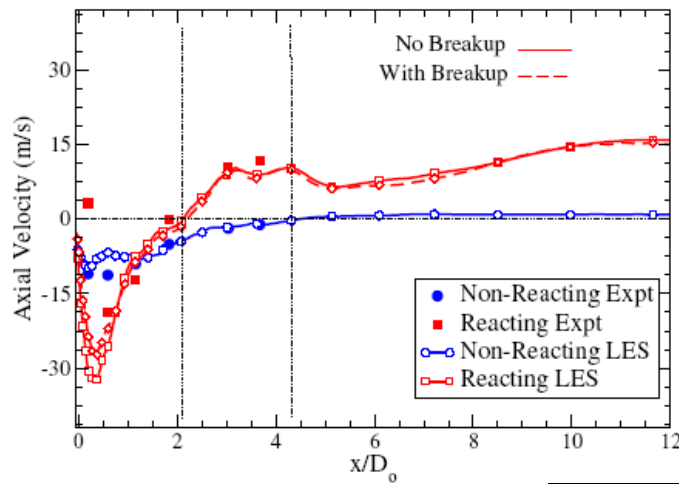


- Particle entrainment by the PVC is effective for dispersion
- VBB and Flame precessing with PVC motion
- Flame index shows presence of premixed & diffusion flames

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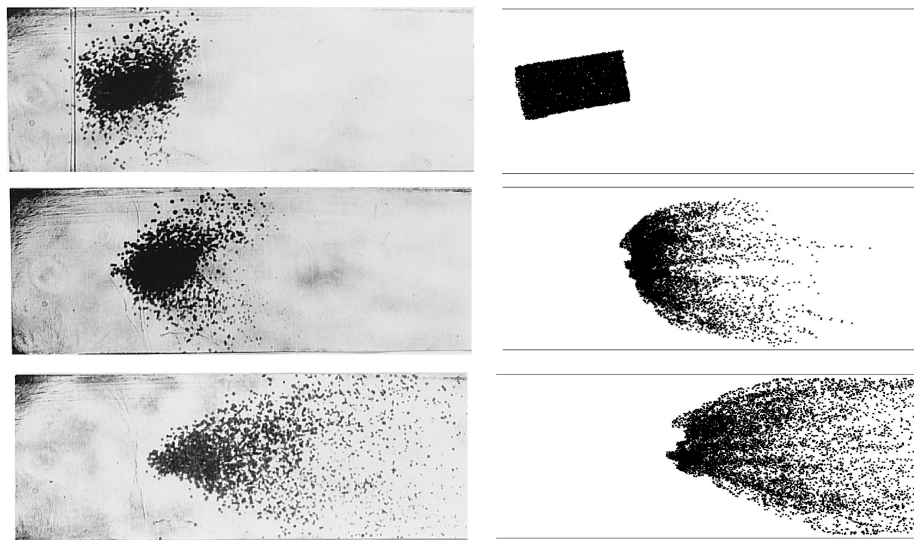
Patel and Menon, 2006, 2008

Effect of Spray Break-up Modeling



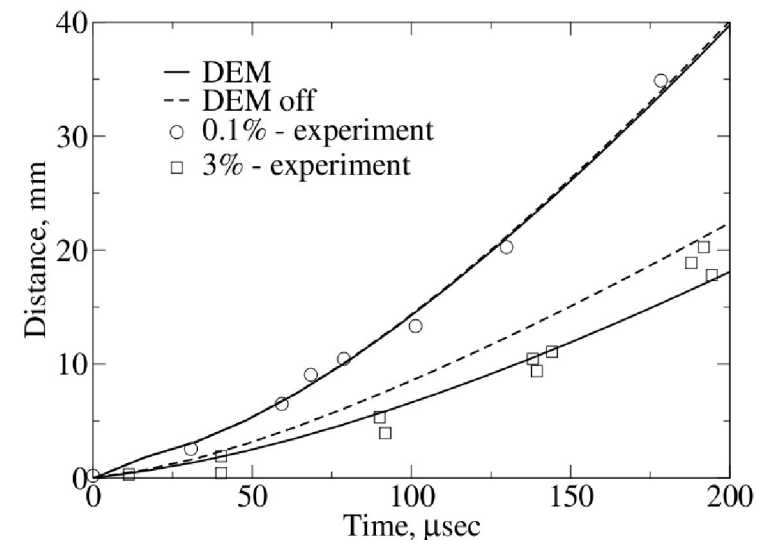
Eulerian Gas Phase Dense Modeling

- Original E-E DEM approach [1] extended to E-L approach [2] to modify gas phase fluxes based on volume fraction loading



Experiment [3]

Simulation [2]



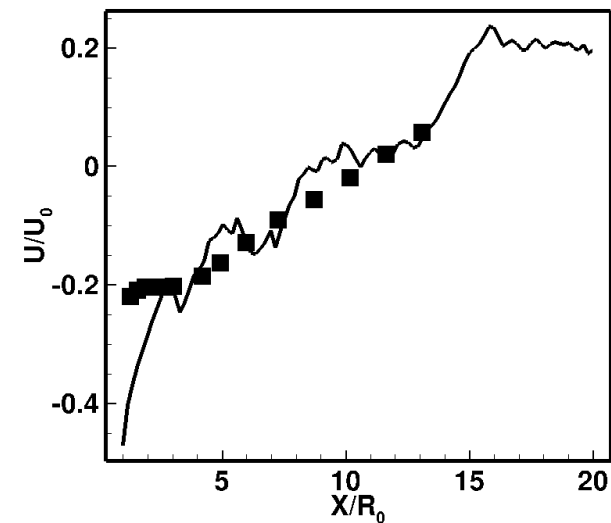
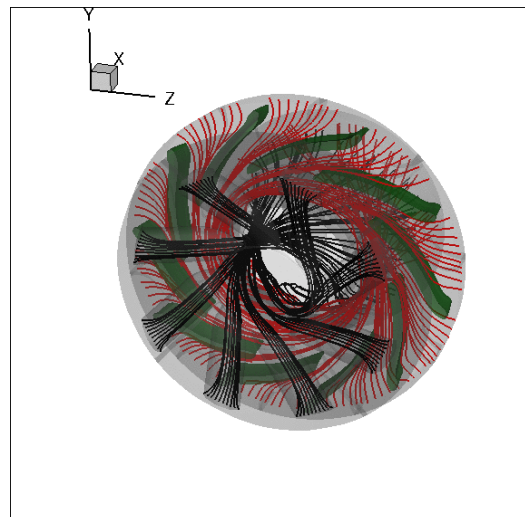
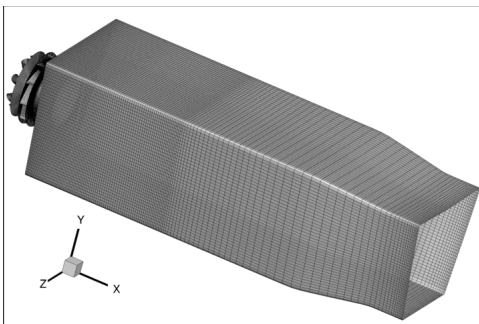
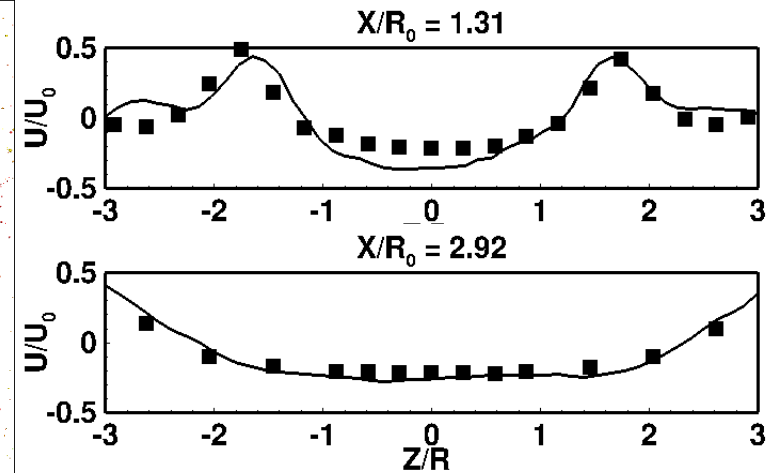
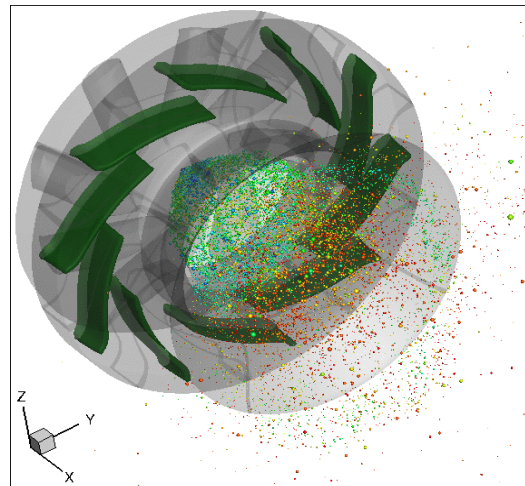
- M=2.8 shock impact on dense cloud of 300 micron particles**
- Dense core of particles form after shock impact**
- Modified Eulerian gas phase fluxes necessary for dense case**

[1] Abgrall and Saurel, J. Comp. Phys., 186, 2003.

[2] Balakrishnan, Nance and Menon, Shock Waves, 20, 2010.

[3] Boiko et al., Shock Waves, 1997

CFM56 Experiments* in Georgia Tech

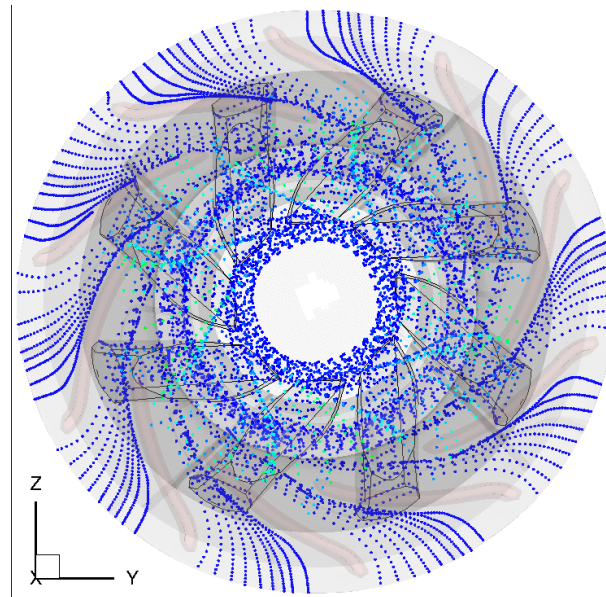
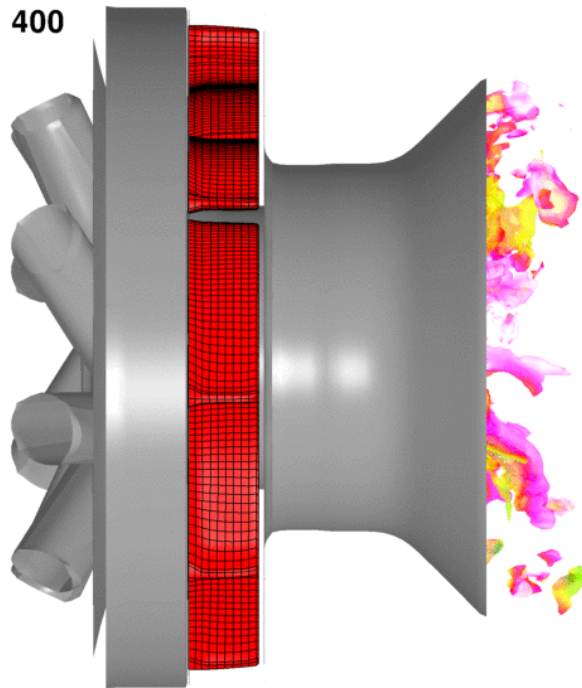
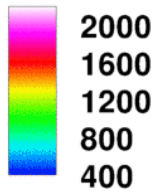


Primary: Red, Secondary: Black

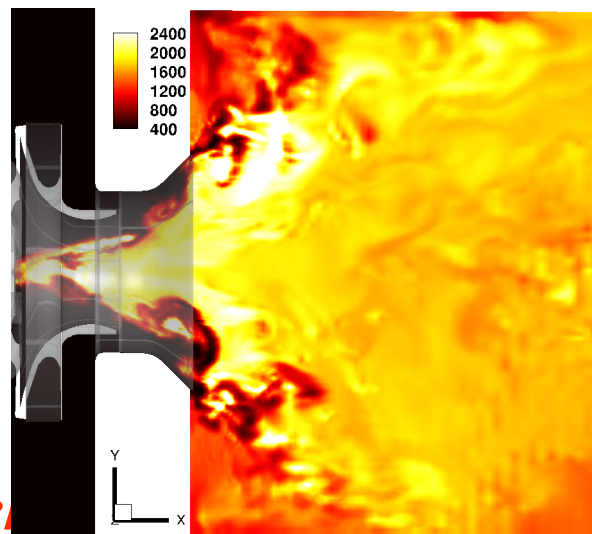
*Suresh Menon, Georgia Tech, ASME-GT2006-90974

Swirling Spray Combustion in CFM56

TEMPERATURE (K)

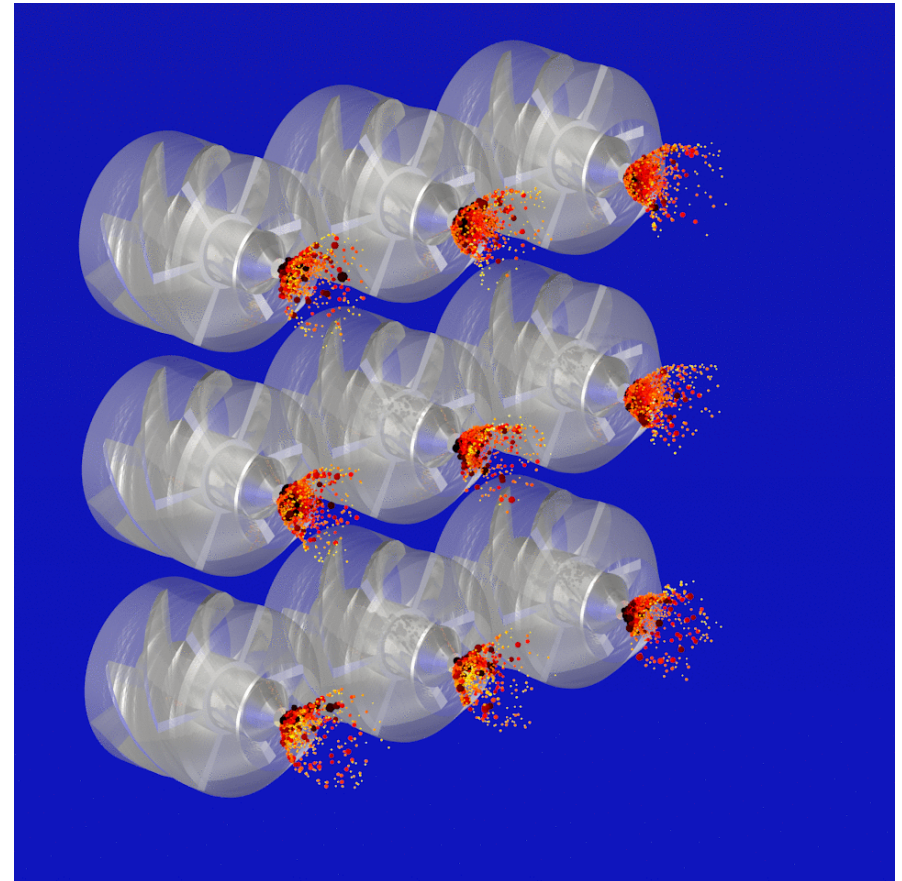
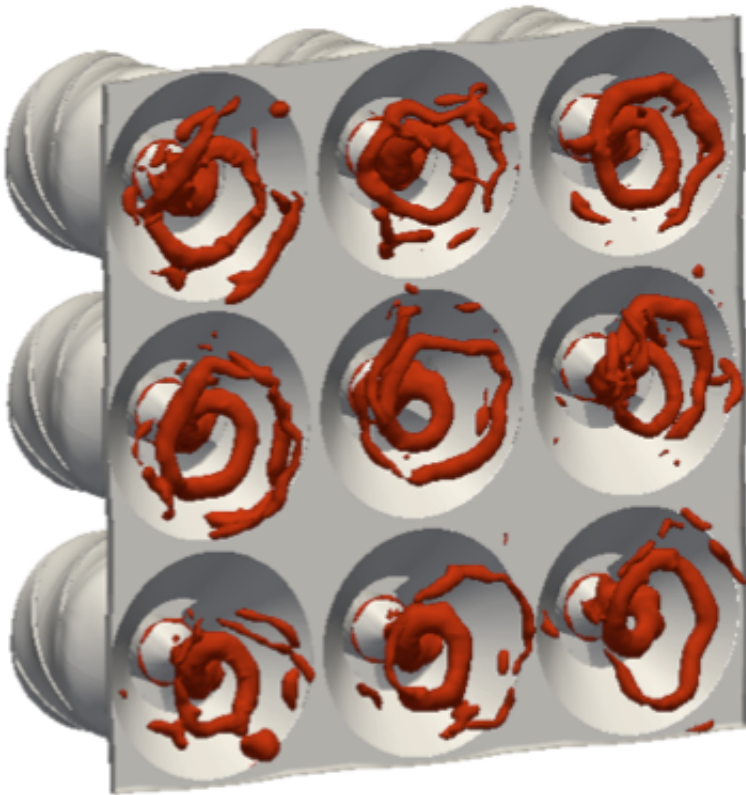


Counter-swirl
streaklines



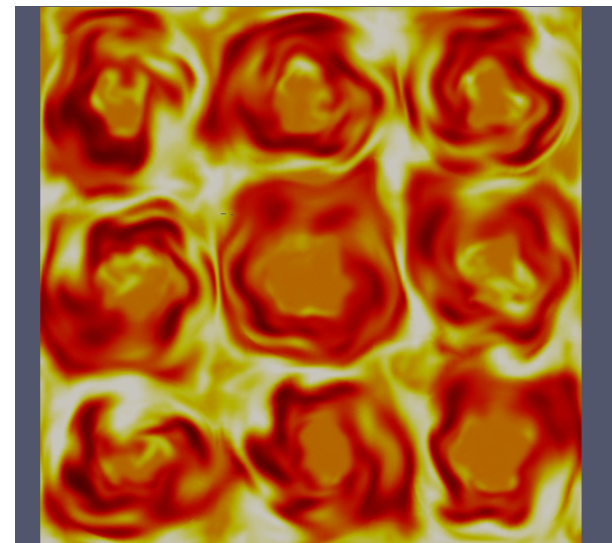
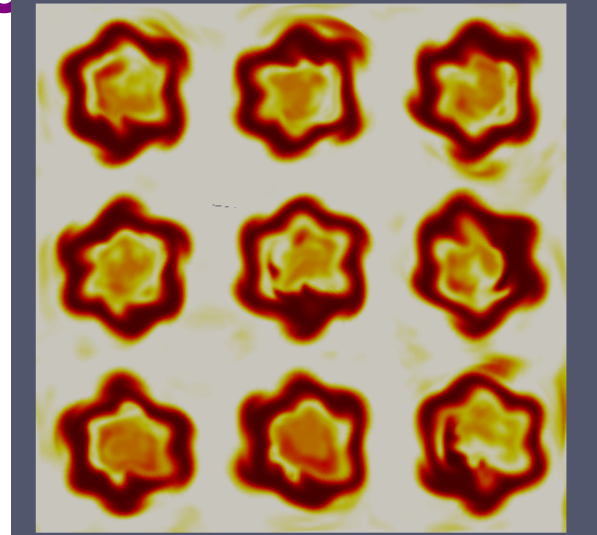
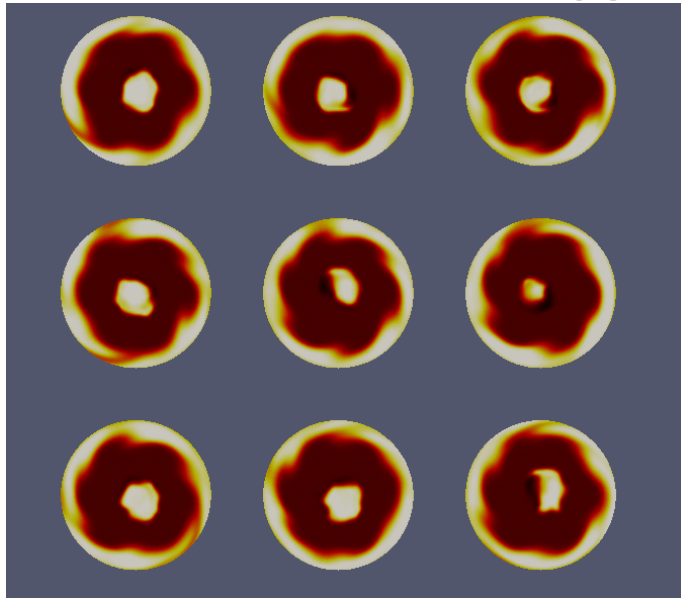
Temperature

9-point LDI at High Pressure



- 10-45M grid with grid refinement
- High pressure 10-27 atm (NASA test rig, Heath et al., 2010)
- *Suresh Menon, Georgia Tech* Kerosene spray with emissions (CO and NO)

9-point LDI: Injector-to-Injector Interactions

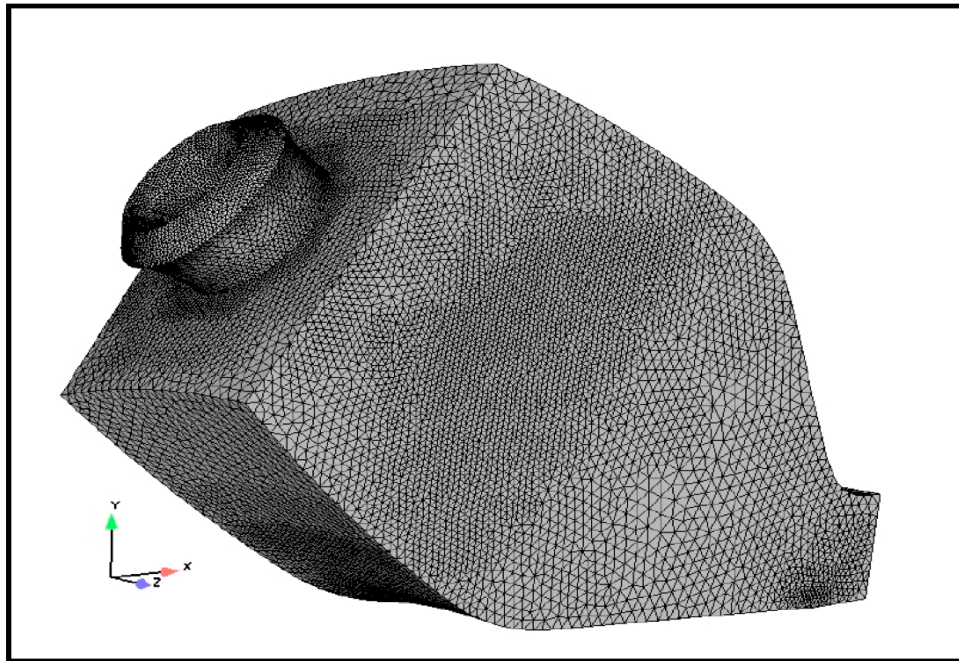


- All have same initial swirl but downstream interactions change mixing and flame structures
- Single injector studies cannot provide insight into this effect

Suresh Menon, Georgia Tech

Gas turbines combustion studies: single sector vs full chamber ?

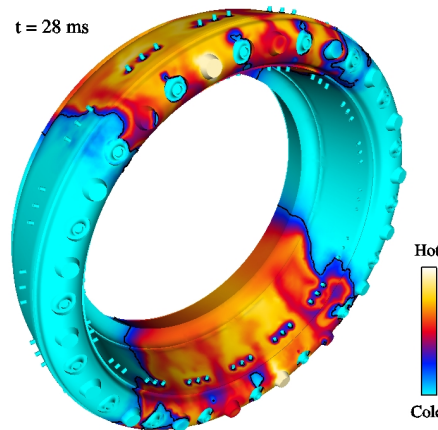
- “Real life”: multi sector (10 to 24) combustion chambers
- Labs: most studies (CFD or experiment) addressing combustion issues are limited to single burners



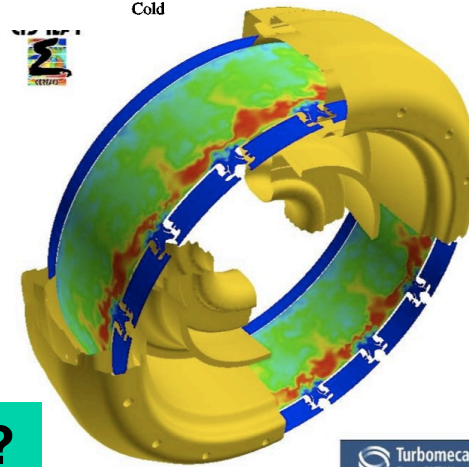
Gas turbines specific mechanisms:

- Certain phenomena found in real gas turbines require LES of full combustion chambers:

– *Ignition*



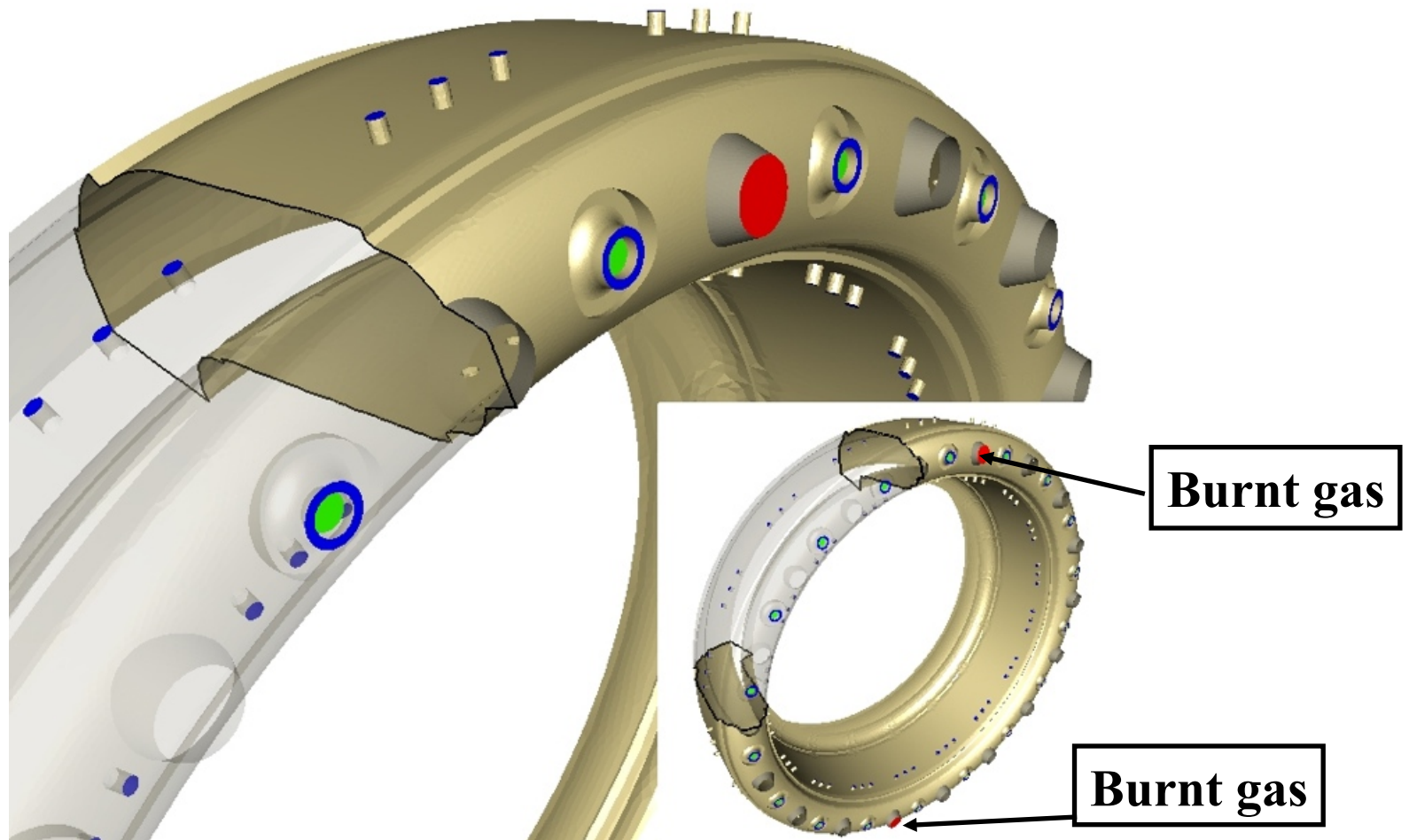
– *Azimuthal modes*



Can LES of a full chamber be performed ?

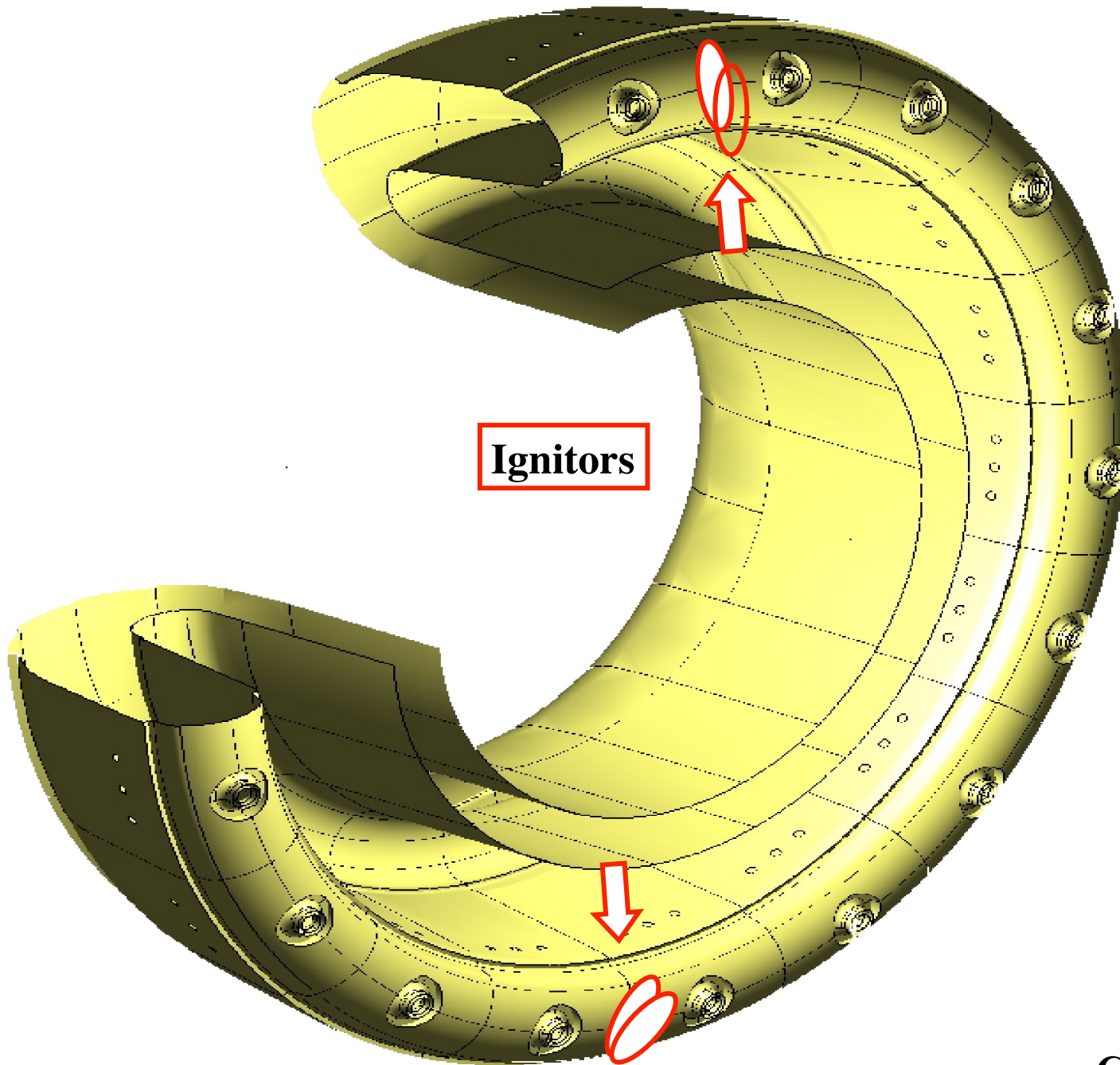
LES of an ignition sequence

- A gas turbine demonstrator: 18 airblast swirled injectors + 2 ignition devices similar to jets injecting hot burnt gases



Suresh Menon, Georgia Tech

Courtesy T. Poinsot



Ignitors

Courtesy T. Poinsot

LES of an ignition sequence

- Numerics:
 - AVBP LES code: 3D turbulent compressible reactive Navier-Stokes solver [2], 2000 processors BG/L
- Chemistry, two-phase flow and flame /turbulence interaction models:
 - WALE model for sub-grid scale viscosity [3]
 - Euler-Euler monodisperse formulation for two-phase flow [6]
 - 19 million tetrahedral cells
 - JP10 1-step mechanism (surrogate for kerosene) [4]
 - Dynamic Flame Thickening TFLES [5]. F goes up to 20.

[2] V. Moureau *et al.*, High-order methods for DNS and LES of compressible multi-component reacting flows on fixed and moving grids, *J. Comp. Phys.*, 2005

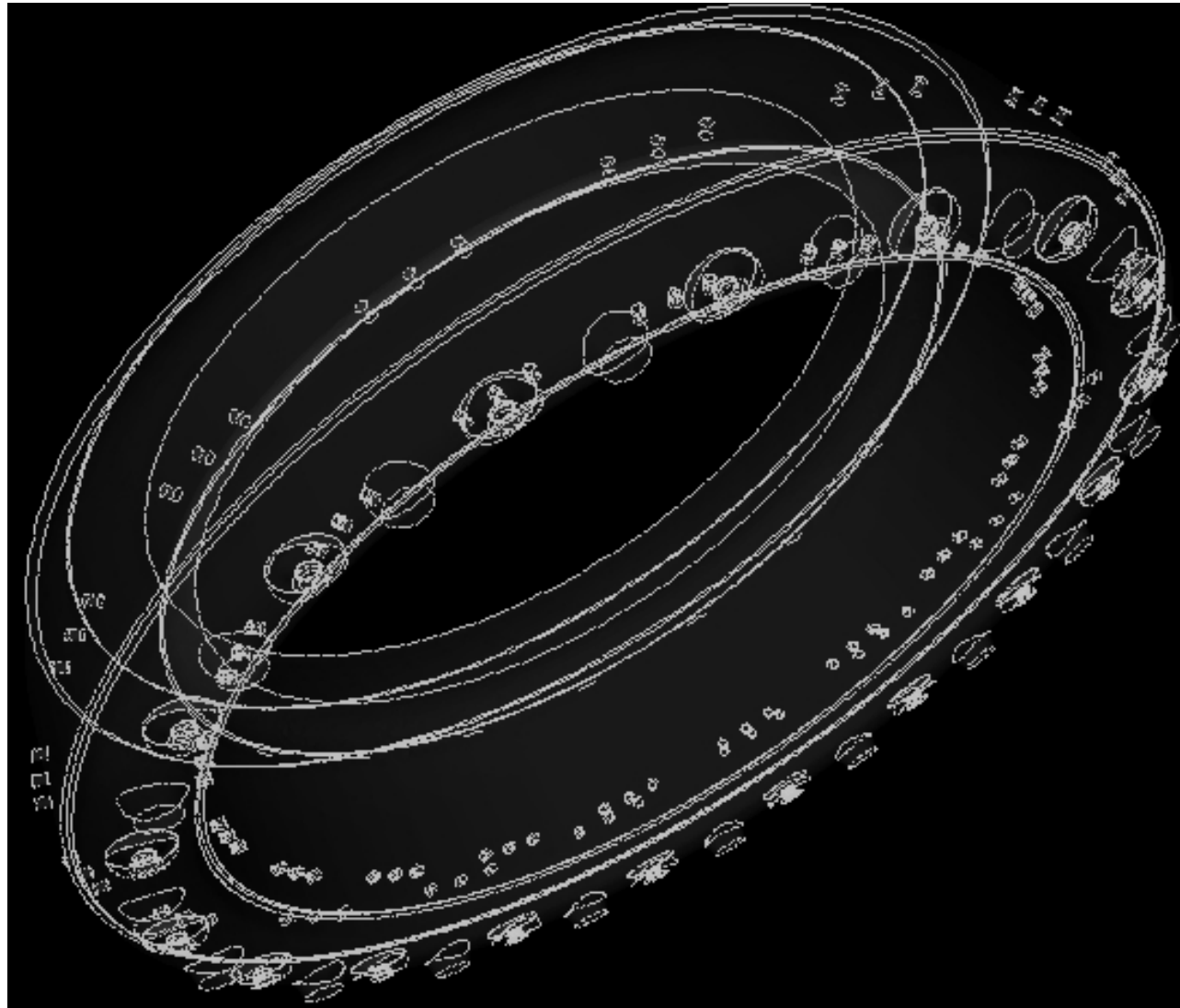
[3] F. Nicoud, F. Ducros, Subgrid-scale stress modelling based on the square of the velocity gradient, *Flow Turb. and Combustion*, 1999

[4] S. Li *et al.*, Chemistry of JP-10 ignition, *AIAA Journal*, 2001

[5] O. Colin, F. Ducros, D. Veynante, T. Poinso, A thickened flame model for large eddy simulations of turbulent premixed combustion, *Phys. Fluids*, 2000

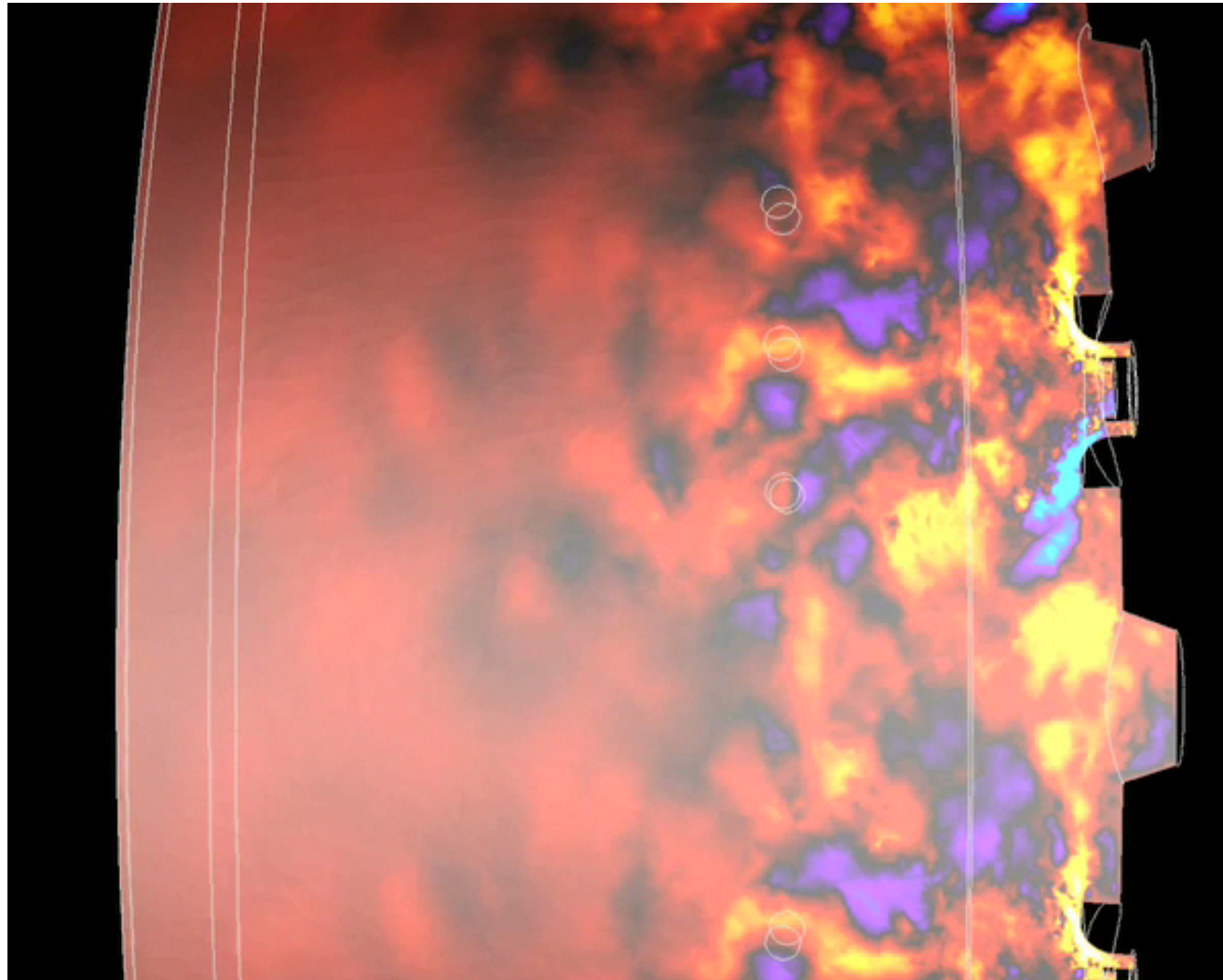
[6] Boileau M., Pascaud S., Riber E., Cuenot B., Gicquel L., Poinso T. and Cazalens M. Investigation of two-fluid methods for Large Eddy Simulation of spray combustion in Gas Turbines. *Flow, Turbulence and Combustion*, 80(3):291-321, (2008).

LES of an ignition sequence



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AIAA CFD for Combustion Modeling



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