Multi-Scale Subgrid Modelling of Turbulent Premixed Combustion at Engine Relevant Conditions

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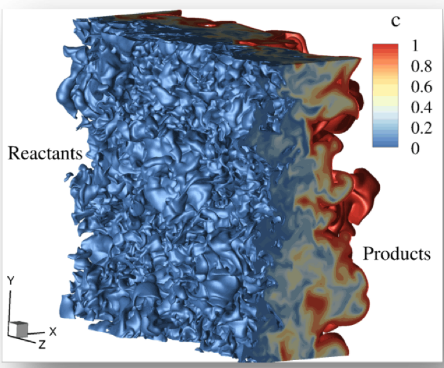
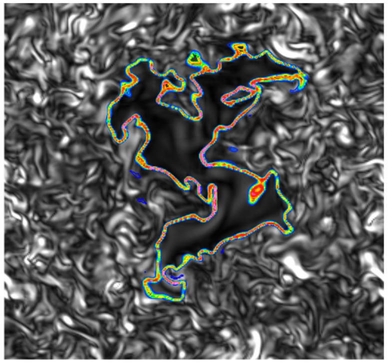
Introduction

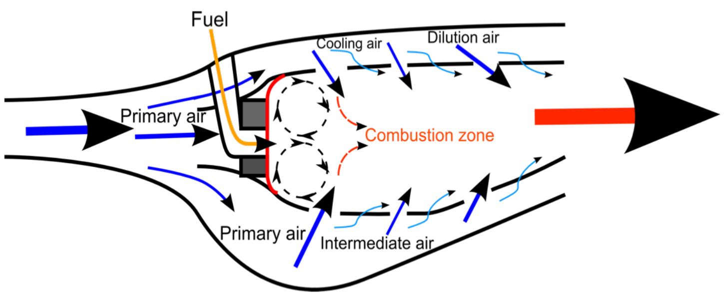
- Turbulent combustion in energy conversion and propulsion devices occur in premixed, non-premixed and partially premixed models
- Multi-scale, non-linear interactions between turbulence, heat-release, acoustics, and boundary conditions.
- Premixed system: variation of equivalence ratio, lean blowout (LBO), combustion instability (CI), extinction-ignition, flashback, partial premixing
- Liquid spray systems involve vaporization and partial premixed combustion, LBO, CI, cold start, altitude restart



Planar flame-turbulence

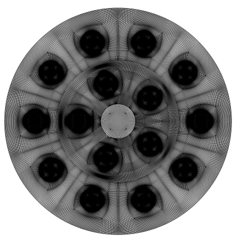


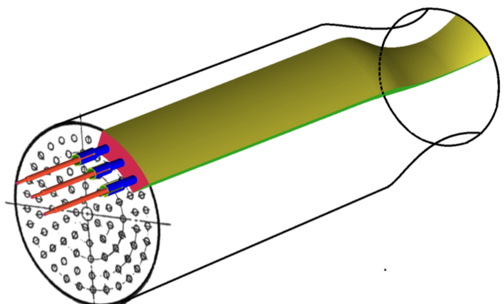
Flame kernel - turbulence



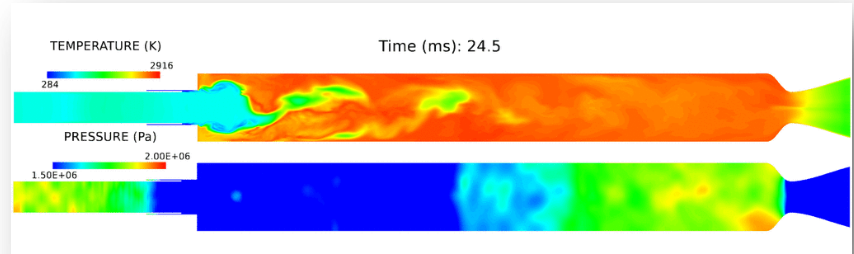
Typical premixed combustor
(*Wikipedia*)

LES in Multi-injector Modeling – Cost and Closure!





2020: Full LRE, 82-injectors, Transv CI
- ~200M cells, coarse-grained LES
- ~ 30-40 days on 10K processors (Est.)
- Real-Gas thermodynamics (DF+VLE)
- PaSR, global 2-step kinetics, K_{sgs}



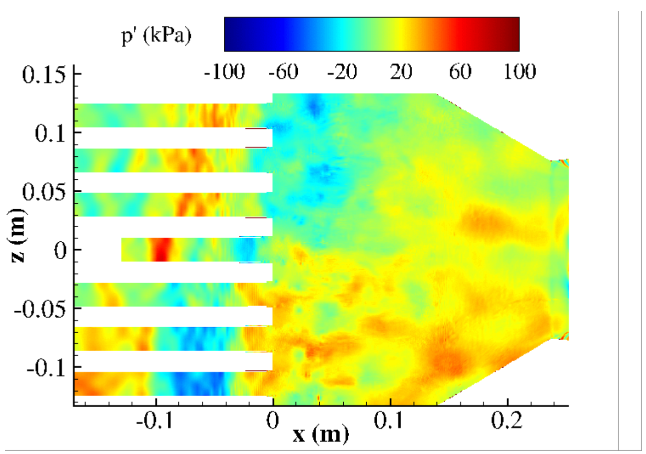
2018 LRE, 15-inectors, Stable/CI
- 36M cells, coarse-grained LES
- 40 hours on 4K processors (3 FTT)
- TPG thermodynamics, 13 MPa
- PaSR, global 2-step kinetics, K_{sgs}

2015: CVRC, 1 injector, Longitudinal CI

1.5M cells, LEMLES+LDKM, 4-step kin., TPG

24 hours on 1.5K cores for 30 cycles of osc.

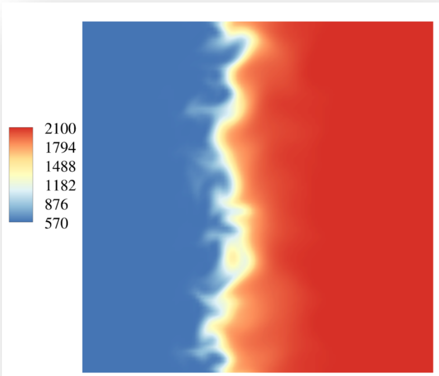
Srinivasan et al., FTAC 2017



2016: TIC, 7 injector, Transverse CI
- 21M cells, two-scale LES, 13 MPa
- ~ 7 days on 2K processors (~5 cycles)
- TPG thermodynamics, 2-step kinetics
- LEMLES + LDKM K_{sgs} models

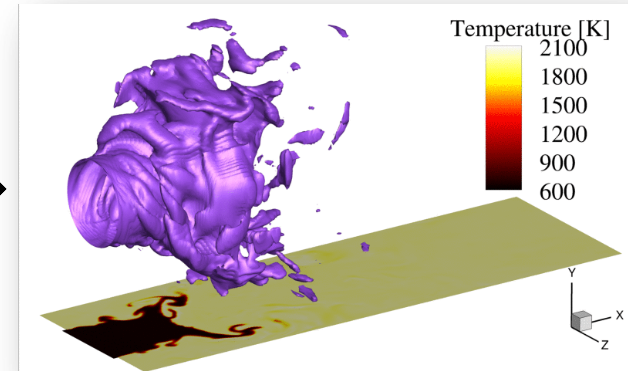
Tudisco and Menon, FTAC 2018

Problems Discussed Here



Turbulent premixed flame interaction at 1 atm

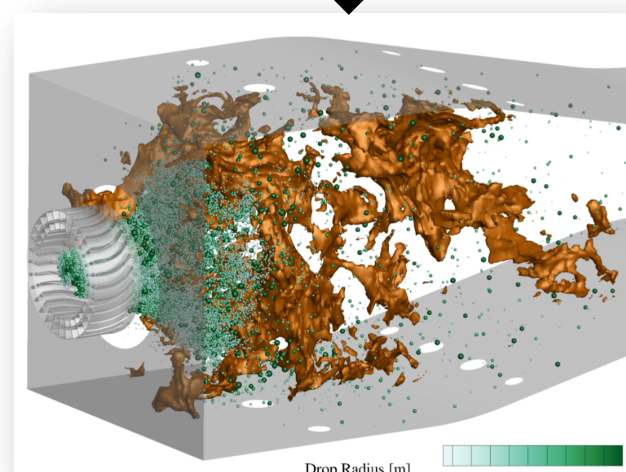
Turbulent premixed flame interaction at 10 atm



Premixed Swirl Combustor (LM6000)

Configuration	Re_t/Re_b	Fuel	Chemistry
Turbulent premixed flame	$O(10^2)$	Methane	4-step and 8-species
LM6000	$O(10^5)$	Methane	73-step and 13-species
UDRI (OEM defined)	$O(10^5)$	Jet Fuel	202-step and 31-species

Towards Engine Relevant Conditions

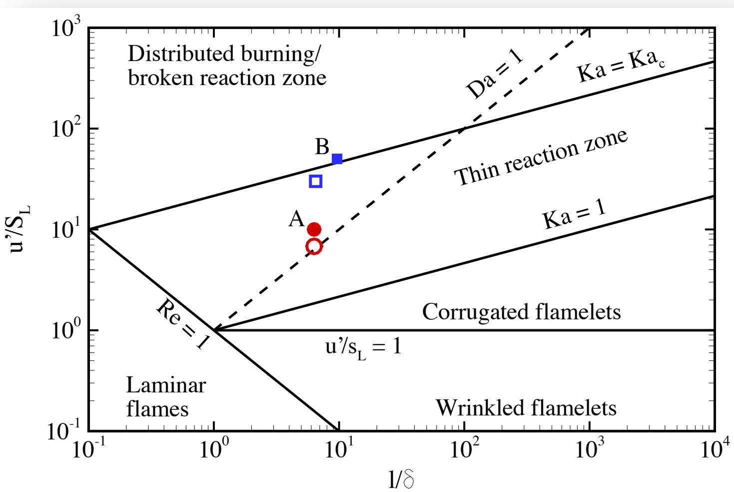


Partially Premixed Combustion with Practical Fuels (UDRI)

Premixed Flame Turbulence Interaction

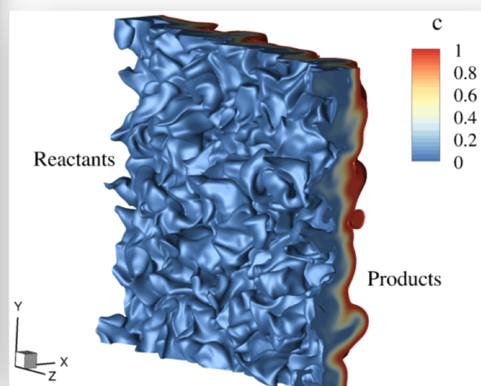
- Freely propagating premixed methane-air flames
- $\varphi = 0.7$, $T_{ref} = 570$ K, $P_{ref} = 1$ atm
- Flames A: TRZ, Flames B: BRZ
- What are the features of interest?

Case	Closure	N_x x N_y x N_z	u'/S_L	l/δ
A_1	DNS	384^3	10	6.2
A_2	LEMLES	96^3	10	6.2
A_3	RRLES	96^3	10	6.2
A_4	QLLES	96^3	10	6.2
B_1	DNS	512^3	50	9.6
B_2	LEMLES	128^3	50	9.6
B_3	QLLES	128^3	50	9.6
B_4	RRLES	128^3	50	9.6

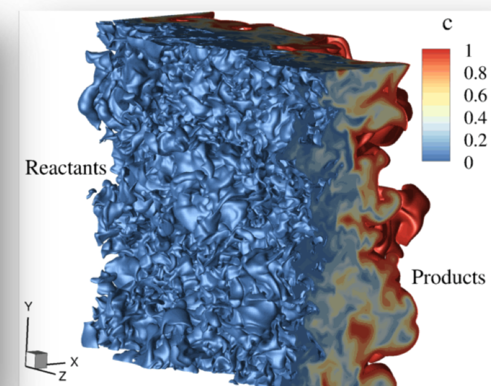


Regime diagram

Flame Structure



Case A_1 ($t = 2\, t_0$)



Case B_1 ($t = 3\, t_0$)

[1]Ranjan et al., CST (2016)

Behavior of SGS Dissipation

- Resolved TKE equation:

$$\frac{\partial \bar{\rho} k}{\partial t} + \frac{\partial \bar{\rho} \widetilde{u_j} k}{\partial x_j} = \alpha_{II} + \alpha_{\nu} + \alpha_{SGS} + \Pi - \epsilon_{\nu} - \epsilon_{SGS}$$

$$\alpha_{II} = -\frac{\partial \bar{p} \widetilde{u_j}}{\partial x_j}, \quad \alpha_{\nu} = \frac{\partial \overline{\tau_{ij}} \widetilde{u_i}}{\partial x_j}, \quad \alpha_{SGS} = -\frac{\partial \tau_{ij}^{SGS} \widetilde{u_i}}{\partial x_j}, \quad \Pi = \bar{p} \frac{\partial \widetilde{u_j}}{\partial x_j}, \ \epsilon_{\nu} = \overline{\tau_{ij}} \widetilde{S_{ij}},$$

$$\epsilon_{SGS} = -\tau_{ij}^{SGS} \widetilde{S_{ij}} \text{ [SGS dissipation]}$$

$$\tau_{ij}^{SGS} = -2 \bar{\rho} \nu_T \widetilde{S_{ij}}, \ \varepsilon_{SGS} = -\tau_{ij}^{SGS} \widetilde{S_{ij}}, \nu_T = C_{\nu} \Delta \sqrt{\mathrm{k}^{sgs}}$$

- Eddy viscosity based closures, $\epsilon_{SGS} \geq 0$
  - Forward cascade of energy from large-scales to small-scales
- In general, space-local and time-local backward transfer of energy from large-scale to small-scales may be observed, referred as **backscatter**
- Investigate SGS energy and scalar dissipations from DNS data

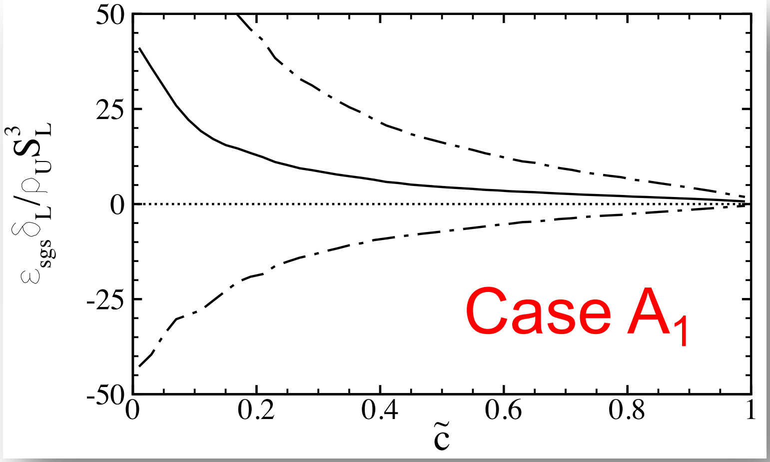
SGS Backscatter: A Priori Analysis

- A priori analysis of DNS backscatter of energy and scalar variance

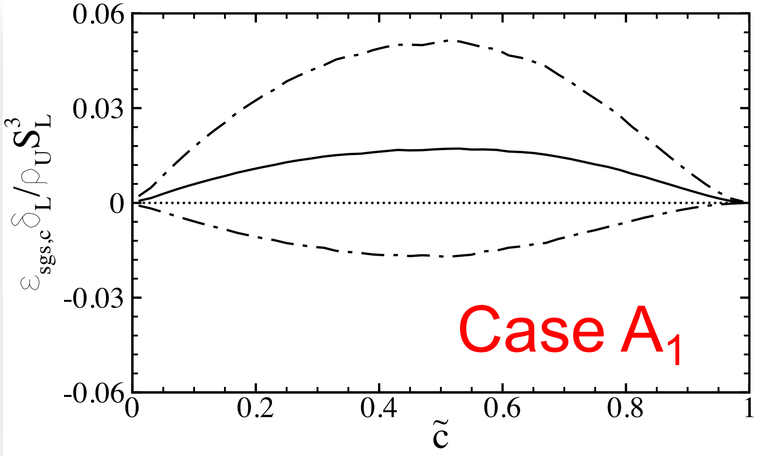
$$\epsilon_{sgs} = -\tau_{ij}^{sgs} \tilde{S}_{ij}$$

$$\epsilon_{sgs,c} = -Y_{ij}^{sgs} \tilde{S}_{ij}$$

- Here, τ_{ij}^{sgs} is SGS stress and Y_{ij}^{sgs} is SGS scalar flux
- Backscatter: $\epsilon_{sgs} < 0$ and $\epsilon_{sgs,c} < 0$
- Solid curve is mean and dash-dotted curve is standard deviation
- Mean is net positive but about 30-40% of backscatter also observed

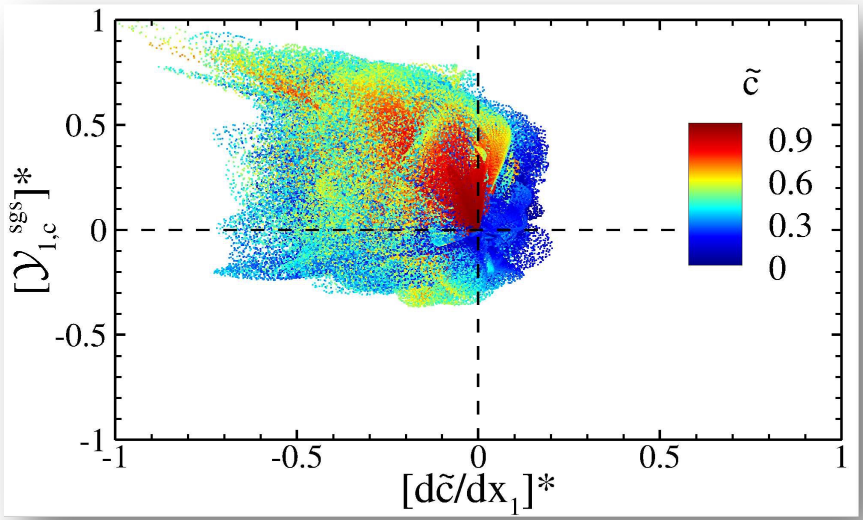


SGS dissipation of TKE

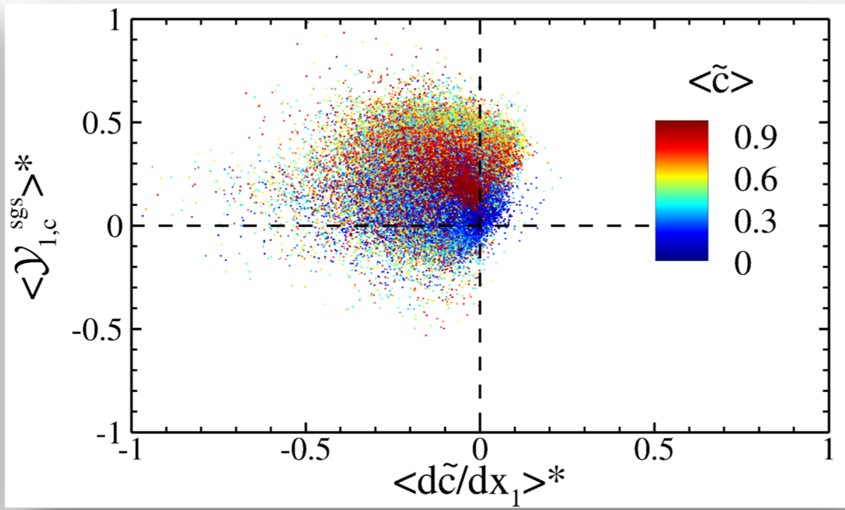


SGS dissipation of scalar variance

Turbulent Scalar Transport



DNS



LEMLES

- Both co- and counter-gradient transport occur
  - Gradient transport only when $-< c'u' > \propto \partial\tilde{c}/\partial x$
  - Most conventional closure models do not account for counter-gradient effects
- Thermal expansion in counter-gradient transport competes with turbulent mixing responsible for co-gradient diffusion [*Wenzel 2000*].

LES Modeling Approaches

Finite-Rate Kinetics LES Equations

- Favre filtered compressible LES Navier-Stokes equations
- Favre filtered LES equations:

$$\frac{\partial \overline{\rho}}{\partial t} + \frac{\partial \overline{\rho}\widetilde{u}_i}{\partial x_i} = 0,$$

$$\frac{\partial \overline{\rho}\widetilde{u}_i}{\partial t} + \frac{\partial}{\partial x_j}\left[\overline{\rho}\widetilde{u}_i\widetilde{u}_j + \overline{P}\delta_{ij} - \overline{\tau}_{ij} + \tau_{ij}^{\mathrm{sgs}}\right] = 0,$$

$$\frac{\partial \overline{\rho}\widetilde{E}}{\partial t} + \frac{\partial}{\partial x_i}\left[\left(\overline{\rho}\widetilde{E} + \overline{P}\right)\widetilde{u}_i + \overline{q}_i - \widetilde{u}_j\overline{\tau}_{ij} + H_i^{\mathrm{sgs}} + \sigma_i^{\mathrm{sgs}}\right] = 0,$$

$$\frac{\partial \overline{\rho}\widetilde{Y}_k}{\partial t} + \frac{\partial}{\partial x_i}\left[\overline{\rho}\left(\widetilde{Y}_k\widetilde{u}_i + \widetilde{Y}_k\widetilde{V}_{i,k}\right) + \mathcal{Y}_{i,k}^{\mathrm{sgs}} + \theta_{i,k}^{\mathrm{sgs}}\right] = \overline{\dot{\omega}}_k \quad k = 1, ..., N_s.$$

- Terms requiring closure:
  - Subgrid-scale terms (superscript ‘sgs’)
  - Filtered reaction-rate term

Modeling of Turbulence-Chemistry Interaction

- Large-scale convection of scalars
  - by coherent structures and mean flow
  - Scalar interface is stretched/wrinkled but not molecularly mixed by these processes
- Other processes needed are
  - Small-scale processes
    - Turbulent mixing by smaller eddies (till Kolmogorov)
    - Molecular diffusion (including differential diffusion)
    - Reaction kinetics and heat release
  - Small-to-large scale coupling
    - Volumetric expansion due to heat release
    - Modification of the velocity field by heat release

Turbulent Combustion Models

- **Models**: assumed flame structure, scale-separation assumption, reduced manifold dimension, chemical source closure, representation of mixing
- Models can be classified in terms of **mixing** and **chemistry**
- **Common closures:**
  - Eddy Dissipation Concept (EDC)[1],
  - Partially Stirred Reactor (PaSR)[2],
  - Thickened Fame Model (TFM)[3],
  - Flamelet[4],
  - Conditional Moment Closure (CMC)[5],
  - Conditional Source Estimation (CSE)[6],
  - Transported PDF[7], Multi-Environment PDF[8],
  - Linear Eddy Model (LEM)[9]
  - One-Dimensional Turbulence (ODT)[10]

Infinitely Fast Chemistry	Bray-Moss-Libby Coherent Flame
Finite-rate w/o molecular mixing	PDF transport
Finite-rate with filtered or model-ed reaction rate	Flamelet model G-equation, G-Z, DTF EBU, FSD, PaSR, RRLES
Finite-rate with molecular mixing	Linear-eddy, ODT

Classification based on mixing and chemistry

[1]Magnussedn (1981), [2]Baudoin et al. (2009), [3]Colin et al. (2000), [4]Ihme & Pitsch (2008), [5]Klimenko & Bilger (1999), [6]Steiner & Bushe (2001), [7]Haworth (2010), [8]Fox (2003), [9]Menon & Kerstein (2011), [10]Echekki et al. (2011),

Employed Modeling Strategies

Features and Capabilities in LESLIE

Main Solver
Compressible
Multi-block Structured FV/FD
Adaptive Mesh Refinement with cut cell

Spatial Schemes
2nd/4th Order (FV & FD)
MUSCL/Central Hybrid
4/5/6 Compact Interpolation
High-order hybrid WENO
High-order Finite Difference

Turbulence Models
One-equation Ksgs dynamic
Smagorinsky dynamic
WALE near wall
K-w-SST, DES near-wall
Hybrid RANS-LES

Turbulence-Chemistry Interaction
Quasi-laminar model
Eddy breakup, Eddy dissipation
Dynamically Thickened Flame
Subgrid Linear Eddy Model
Flamelet-Progress Variable

Temporal Schemes
O(2) Explicit
2nd-4th Order Explicit Runge-Kutta
Implicit and Pre-conditioning

Thermodynamics
CPG, TPG, Real Gas
Vapor-liquid Equilibrium
Mie-Grunesen
JWL, Hayes, Abel-Nobel

Transport and Kinetics
Power law, Sutherland
Mixture averaged
Multi-species Finite-Rate
CANTERA, CHEMKIN

Boundary Conditions
Characteristic Inflow/Outflow
Supersonic
Sponge Layers
Reactive Wall Treatment
Mass Ejection

Particle Phase
Solid/liquid reactive particles
Breakup, collision, compressibility,
Soot, aerosol (MOMIC)
Eulerian-Eulerian Eulerian-Lagrangian
Two-Phase Dense Phase Solver
Peridynamics Model for microstructure

Data Analysis
Turbulent statistics
Flame-Flow-Acoustic
Analysis, UDFs

FSI
Immersed BCs
HS, void
Heat Transfer
Microstructure

Black: Production Code
Red: Current Code Use

Subgrid Models Investigated in Same Code

Modeling Type	Paradigm	Scalar Mixing	Reaction-rate
FRC-DNS	Finite-rate kinetics	-	-
FPV-DNS	Low dimensional manifold	-	-
LEMLES	Finite-rate kinetics/multi-scale	LEM	LEM
Single/Multi-level RRLES	Finite-rate kinetics/multi-scale	Eddy diffusivity	LEM
FPV-LES	Low dimensional manifold	Eddy diffusivity	Beta-PDF
SDR-LES	Low dimensional manifold	Eddy diffusivity	Modeled SDR
FPV-RRLES	Low dimensional manifold	Eddy diffusivity	LEM
SDR-RRLES	Low dimensional manifold	Eddy diffusivity	LEM

LEMLES Approach

- Exact species transport equation in the modified form:

$$\rho\frac{\partial Y_k}{\partial t}+\rho\left[\widetilde{u}_i+(u_i')^R+(u_i')^S\right]\frac{\partial Y_k}{\partial x_i}+\frac{\partial}{\partial x_i}\left(\rho Y_k V_{k,i}\right) = \dot{\omega}_k$$

$$u_i=\widetilde{u}_i+(u_i')^R+(u_i')^S$$

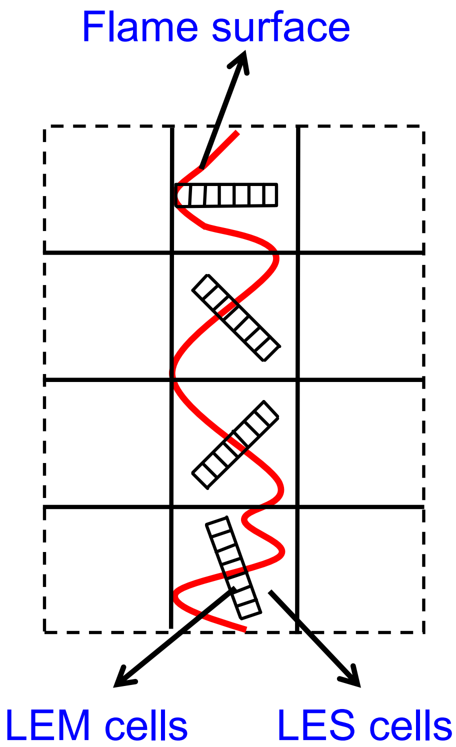
- LEMLES[1] uses two-scale decomposition to solve for scalars

Subgrid scale (Eulerian, Stochastic 1D)

$$Y_k^*-Y_k^n=\int_t^{t+\Delta t_{\text{LES}}}-\frac{1}{\rho}\left[\rho\left(u_i'\right)^S\frac{\partial Y_k^n}{\partial x_i}+\frac{\partial}{\partial x_i}\left(\rho Y_k V_{i,k}\right)^n-\dot{\omega}_k^n\right]dt'$$

Resolved scale (Lagrangian, Deterministic, 3D)

$$\frac{Y_k^{n+1}-Y_k^*}{\Delta t_{\text{LES}}}=-\left[\widetilde{u}_i+(u_i')^R\right]\frac{\partial Y_k^n}{\partial x_i}$$



- Filtered species obtained from the subgrid LEM field
- Reaction rate in subgrid domain requires no closure
- Model more accurate in high Re LES

[1]Menon & Kerstein (2011); [2]Kerstein, CST (1988); [3]Gonzalez-Juez et al., PECS (2017)

Well known Limitations of LEMLES

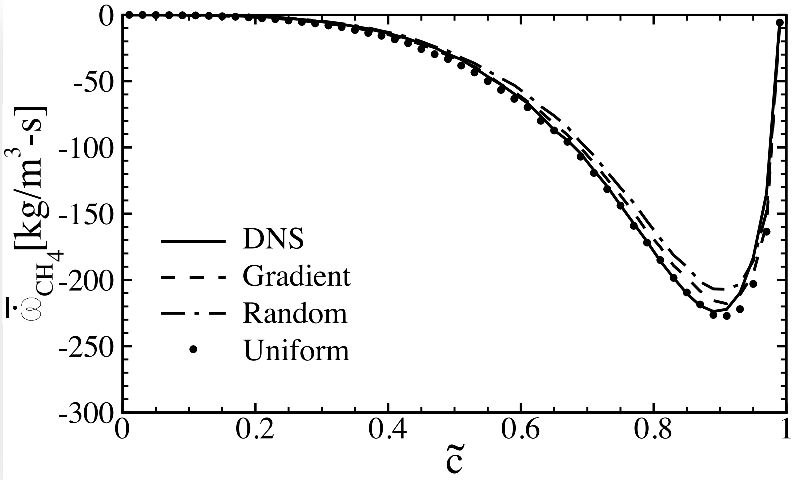
- Sub-grid resolution constraints can lead to artificial numerical diffusion
- Large-scale laminar diffusion is ignored compared to turbulent diffusion
  - asymptotic convergence to low Re molecular diffusion needed
- Triplet mapping is discrete and instantaneous whereas turbulent mixing is continuous and has a finite time-scale – sensitivity primarily at low Re
- Current LEMLES assumes pressure to be constant but can be relaxed
  - Necessary for high Mach number flows
  - Need to account for sub-grid shock motion
- New approach developed to address some of these limitations but brings some other constraints (RRLES)

RRLES v/s LEMLES

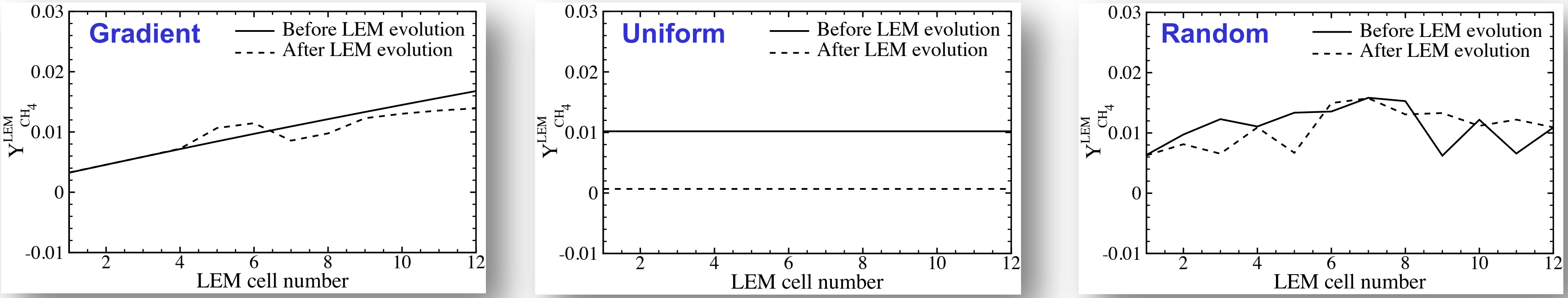
- Solve convention scalar transport equations along with LES
- Conventional SGS closure for scalar subgrid flux
- Reaction Rate obtained using subgrid LEM locally
- RRLES advantages
  - molecular diffusion recovered in the limit of laminar and DNS limit
  - Reaction rate within the subgrid LEM requires no explicit closure
- RRLES disadvantages
  - cannot capture counter-gradient turbulent scalar transport
  - Subgrid initialization recovers only mean scalar features

Reconstruction of LEM Fields

- Three strategies considered so far:
  - Use resolved scalar gradient
  - Uniform: No stirring can occur
  - Random using Gaussian distribution with algebraic model for variance
- Posteriori assessment showed gradient strategy is better but this needs more studies
- Higher moments may need to be considered



Conditional variation of filtered reaction rate of fuel w.r.t. progress variable



Initially reconstructed and evolved LEM solution

Single Grid RRLES Formulation

- Subgrid scalar flux modeled using gradient eddy diffusivity approach:

$$\mathcal{Y}_{k,i}^{\mathrm{sgs}} = -\overline{\rho} D_t \frac{\partial \widetilde{Y}_k}{\partial x_i}$$

- Species transport equations expressed as:

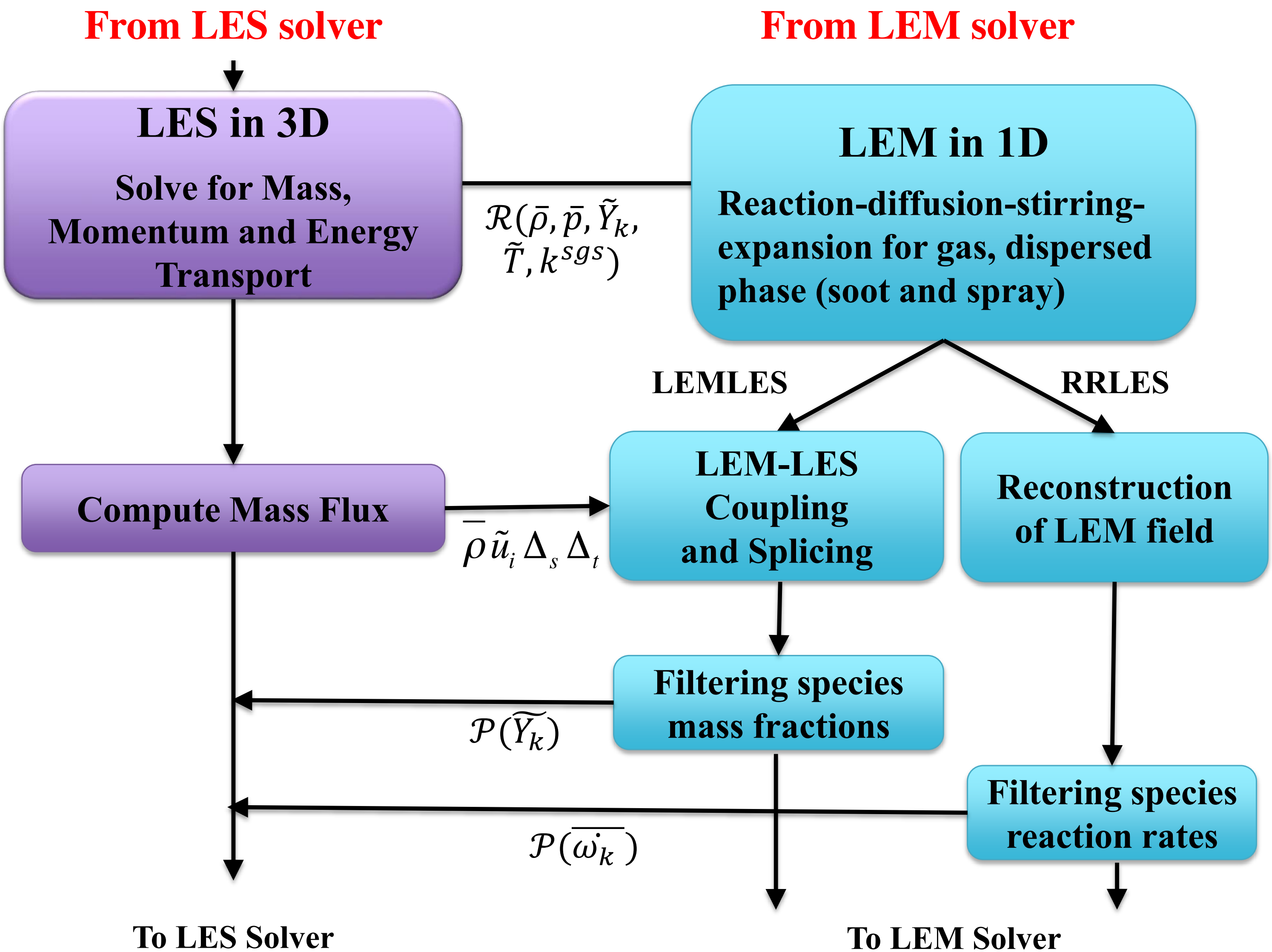
$$\frac{\partial \overline{\rho}\widetilde{Y}_k}{\partial t} + \frac{\partial}{\partial x_i}\left[\overline{\rho}\left(\widetilde{Y}_k\widetilde{u}_i - \frac{\nu_t}{Sc_t}\frac{\partial \widetilde{Y}_k}{\partial x_i}\right)\right] = -\frac{\partial}{\partial x_i}\left[\overline{\rho}\widetilde{Y}_k\widetilde{V}_{k,i}\right] + S_k \quad k = 1, 2, \ldots, N_{\mathrm{s}}$$

$$S_k = -\frac{\partial \theta_{k,i}^{\mathrm{sgs}}}{\partial x_i} + \overline{\dot{\omega}}_k$$

Explicitly modeled LEM term

[1]Ranjan et al., CST, 188 (2016)

LEMLES v/s Single-Level RRLES



FPV-LES Approach

- Filtered equation for progress variable (c)[1-3]:

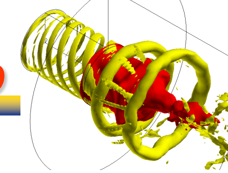
$$\frac{\partial \bar{\rho}\tilde{c}}{\partial t} + \nabla.(\bar{\rho}\tilde{u}_i\tilde{c}) = \nabla.(\bar{\rho}(\tilde{\alpha}_c + \alpha_T)\nabla\tilde{c}) + \bar{\rho}\bar{\dot{\omega}}_c$$

- Subgrid fluctuations in *c* is accounted by:

$$\tilde{Y}_k = \int Y_k(c)\,\tilde{P}(c)dc$$

- Here, $Y_k(c)$, $T(c)$, and $\bar{\dot{\omega}}_c(c)$ are obtained from flamelet library and $\tilde{P}(c)$ is assumed to be a beta PDF[4]
- Compressible flamelet models also exist but the current implementation is still the classical one

[1]Oijen & de Goey (2000); [2]Pierce & Moin (2004); [3]Oijen et al. (2007); [4]Cook et al. (1994)



SDR-LES Approach

- Filtered transport equation for a progress variable

$$\frac{\partial \bar{\rho}\tilde{c}}{\partial t} + \nabla.(\bar{\rho}\tilde{\boldsymbol{u}}\tilde{c}) = \nabla.[\bar{\rho}(\bar{D} + D_T)\nabla\tilde{c}] + \bar{\dot{\omega}}_c$$

- The reaction rate closure is attained through an algebraic model:

$$\bar{\dot{\omega}}_c = \frac{2}{2C_m - 1}\bar{\rho}\widetilde{N}_c, \text{ where } \widetilde{N}_c = \bar{D}\,\nabla\tilde{c}.\nabla\tilde{c} + \tilde{\epsilon}_c$$

- Different approaches exist for modeling of SGS scalar dissipation rate:

Conventional[1]

$$\tilde{\epsilon}_c = \bar{D}_{\mathrm{T}}\,\nabla\tilde{c}.\nabla\tilde{c}$$

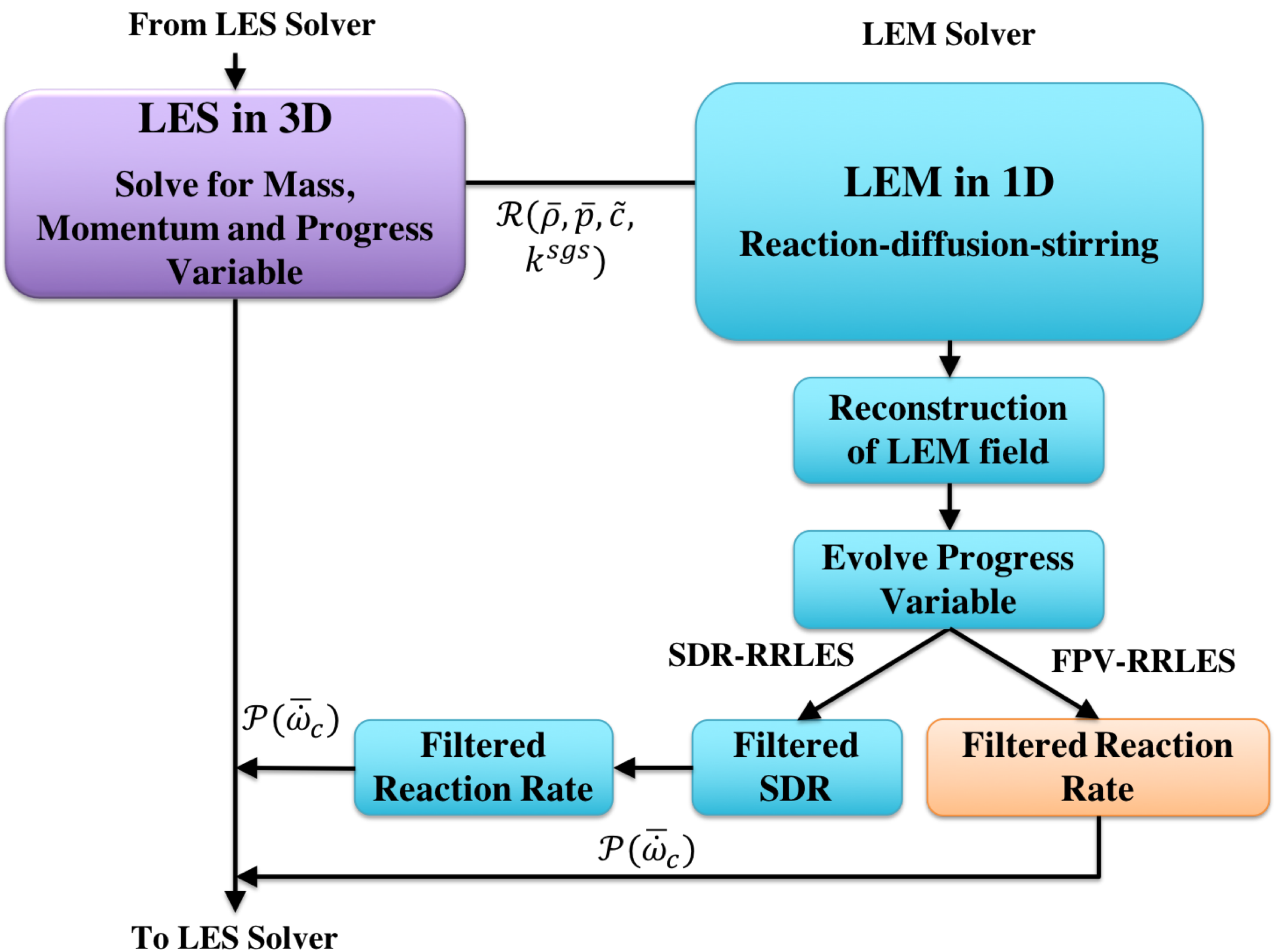
Extended[2,3]

$$\tilde{\epsilon}_c = \mathcal{F}\left[2K_c\frac{S_L}{\delta_{th}} + (C_3 - \tau C_4 Da_\Delta)\left(\frac{2u'}{3\Delta}\right)\right]\frac{\sigma_{c,sgs}^2}{\beta_c}$$

- Conventional closure is used but extended closure is being evaluated for $\tilde{\epsilon}_c$
- Extended model involves parameters some of which can be tuned or obtained dynamically and it involves flame speed, flame thickness, local SGS velocity scale

[1]Girimaji & Zhou (1996), [2]Gao et al. (2014), [3]Mao et al. (2014)

FPV-RRLES and SDR-RRLES Workflow



RRLES of Flame-Turbulence

- Interaction of premixed methane flame with decaying isotropic turbulence[1] ($\phi = 0.8, T_{ub} = 570$ K)

Case	Closure	N_x x N_y x N_z	u'/S_L	l/δ
A_1	DNS	384^3	10	6.2
A_2	LEMLES	96^3	10	6.2
A_3	RRLES	96^3	10	6.2
A_4	QLLES	96^3	10	6.2
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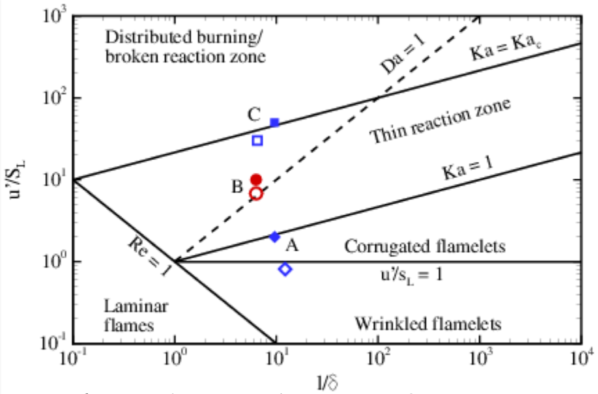
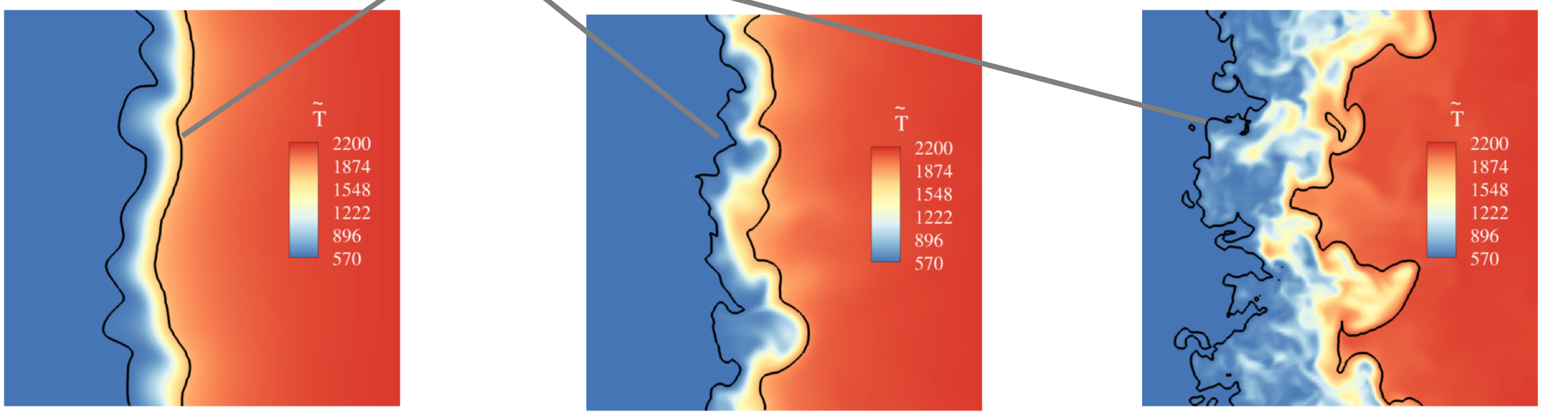


Flame brush: isolines of $\tilde{c} = 0.01$ and $\tilde{c} = 0.99$



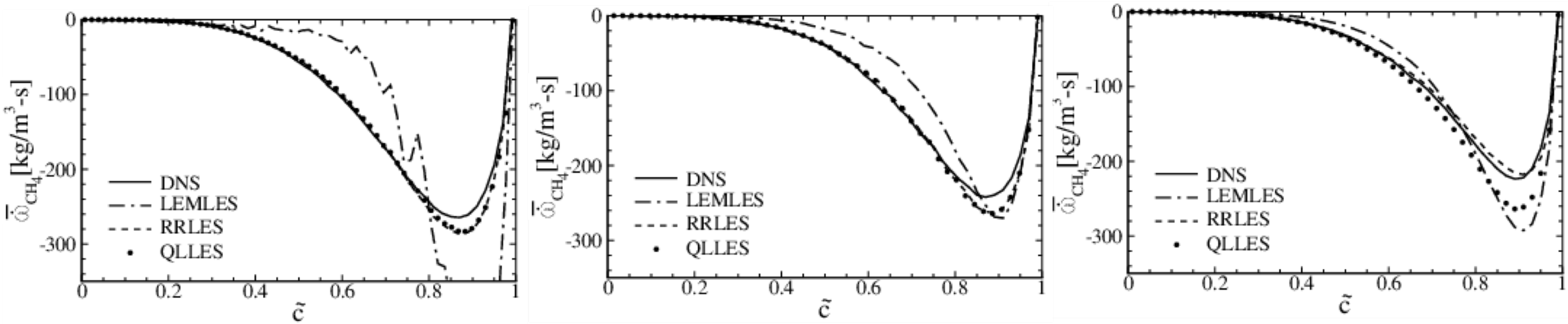
Corrugated flamelet[1] *Thin reaction zone[1]* *Broken reaction zone[1]*

*Ranjan R, Muralidharan B, Nagoaka, Y., and Menon S, CST, 2016, VOL. 188, NO. 9, 1496–1537

RRLES of Flame-Turbulence Interactions

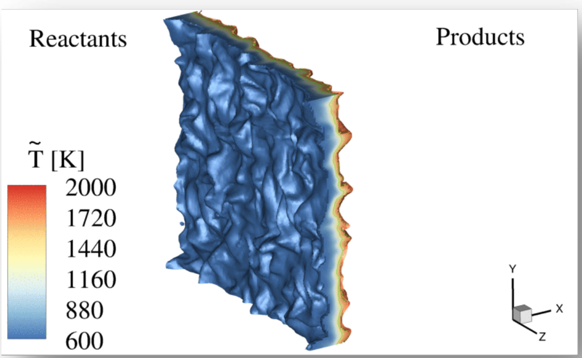
- Conditioned mean of Methane reaction rate

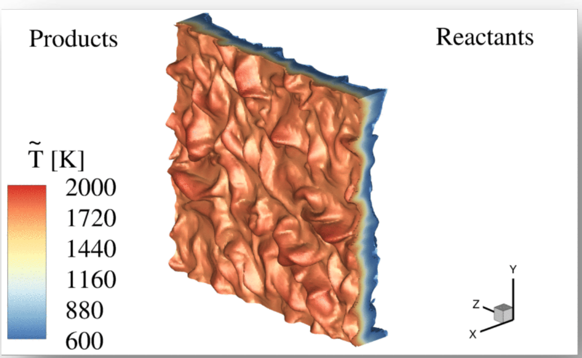
Corrugated flamelet *Thin reaction zone* *Broken reaction zone*

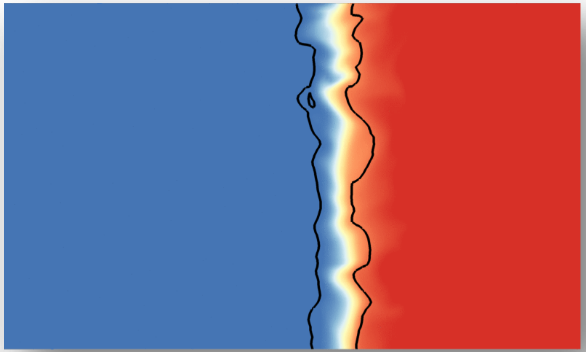


- Lower Re
  - RRLES approach asymptotes to QLLES (Quasi Laminar)
  - Linear Eddy Model has a known problem at low Re
- Higher Re (but is still relatively low) - RRLES predicts better reaction rates

Comparison of Different Closures







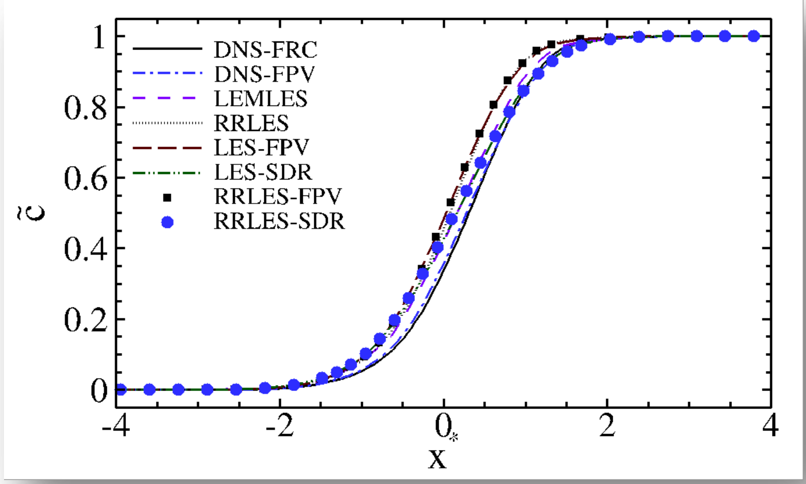
Focus on TRZ Flame Only

- TRZ regime $(\frac{u'}{S_L} = 10, \frac{l}{\delta} = 10)$, φ = 0.8, T_{ref}= 570 K, P_{ref} = 1 atm
- Eight simulations performed with 2 DNS reference for FRC and FPV approaches
- 12 LEM cells per LES cell considered for multi-scale approaches
- 4-step and 8-species mechanism considered for FRC, and FPV table generated using same mechanism
- Results compared after 2 eddy turnover time (τ_0)

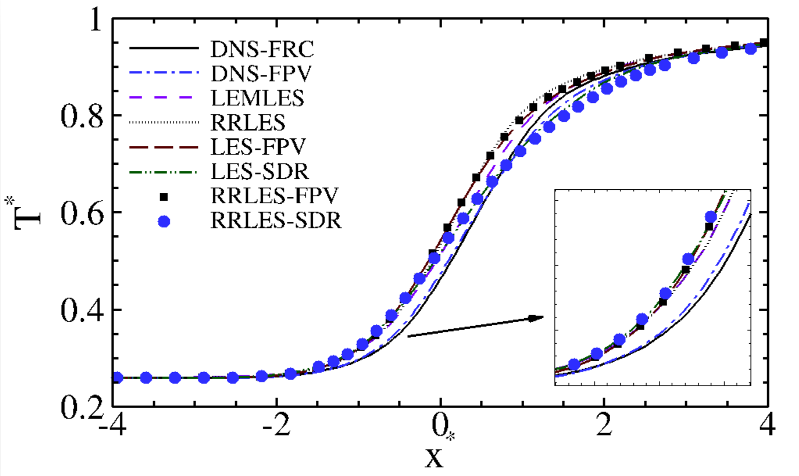
Case	N_x x N_y x N_z	CPU Hrs for $2\tau_0$
DNS-FRC	384^3	XX
DNS-FPV	384^3	XX
LEMLES	96^3	1972
RRLES	96^3	1861
LES-FPV	96^3	164
LES-SDR	96^3	148
RRLES-FPV	96^3	445
RRLES-SDR	96^3	445

Averaged Flame Structure

- Averaged flame structure obtained by averaging along transverse directions
- Overall, all methods capture mean flame structure reasonably well, with differences evident in preheat and post-flame regions
- Quantitative differences exist in mean flame location and thickness
  - Effect of chemistry modeling
  - Effect of turbulence-chemistry modeling



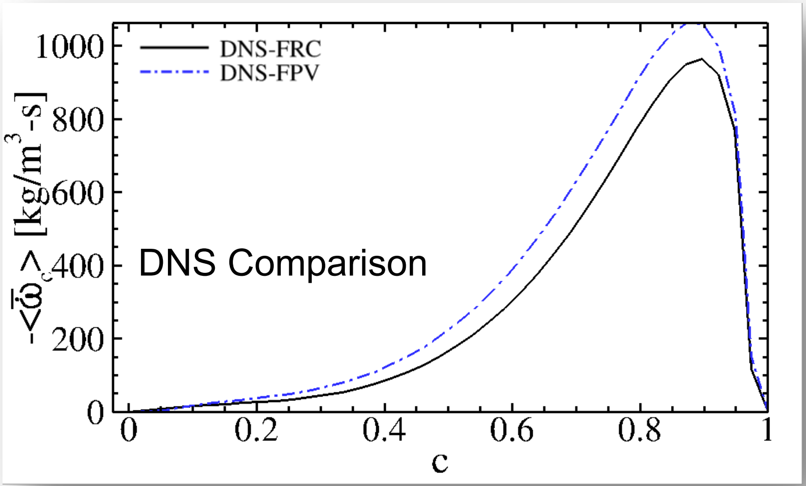
Progress Variable



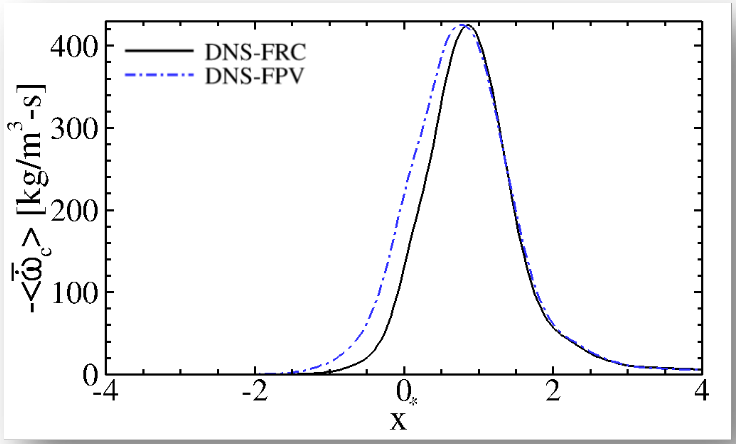
Temperature

Statistics of Filtered Reaction Rate

- **Effect of chemistry modeling**
  - DNS-FPV show higher RR in the prog. var. conditional space compared to DNS-FRC
  - Physical space RR can be considered a manifestation of the prog. var. space RR



Reaction Rate (RR) in Prog. Var Space

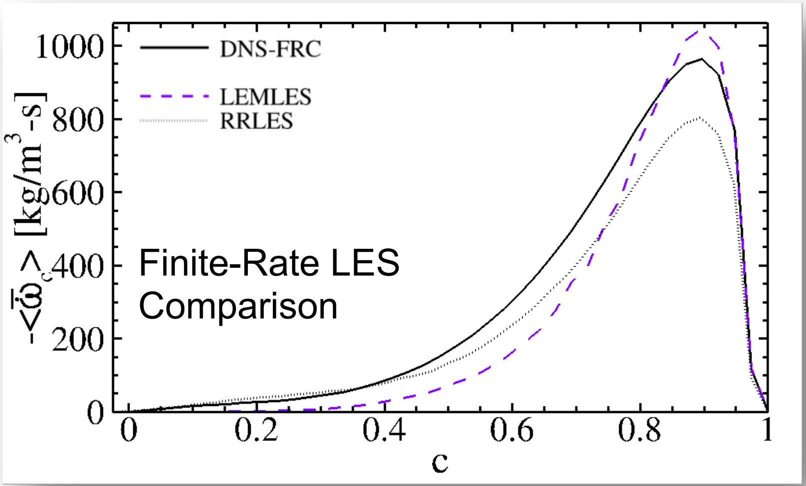


Reaction Rate (RR) in Physical Space

[1]Ma et al., CF 161, (2014), [2]Gao et al., CST 186, (2014)
[3]Ranjan et al., CST 188, (2016)

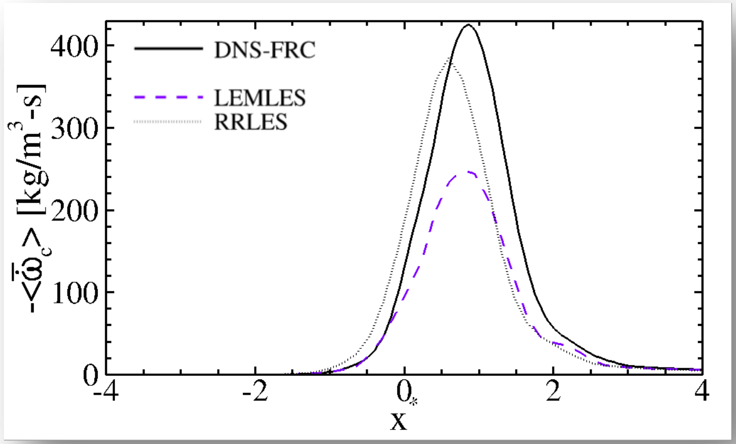
Statistics of Filtered Reaction Rate

- Effect of chemistry modeling
  - DNS-FPV show higher RR in the prog. var. conditional space compared to DNS-FRC
  - Physical space RR can be considered a manifestation of the prog. var. space RR
  -



Reaction Rate (RR) in Prog. Var Space

- **Effect of turbulence-chemistry modeling**
  - RRLES predictions better than LEMLES[3]

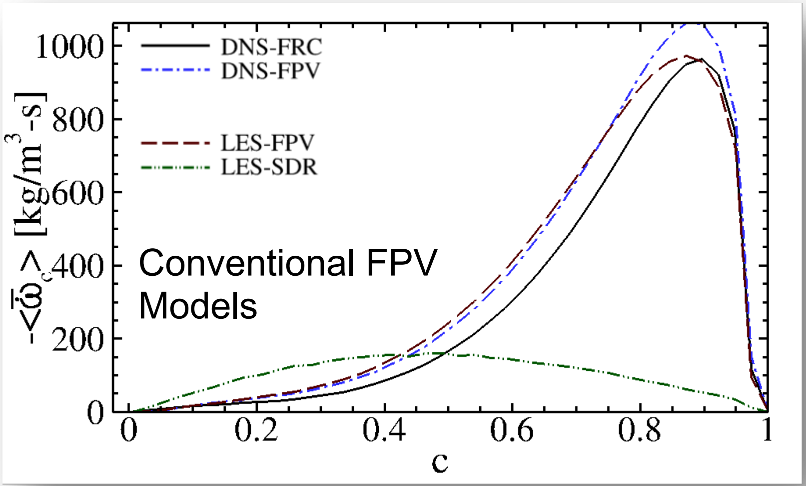


Reaction Rate (RR) in Physical Space

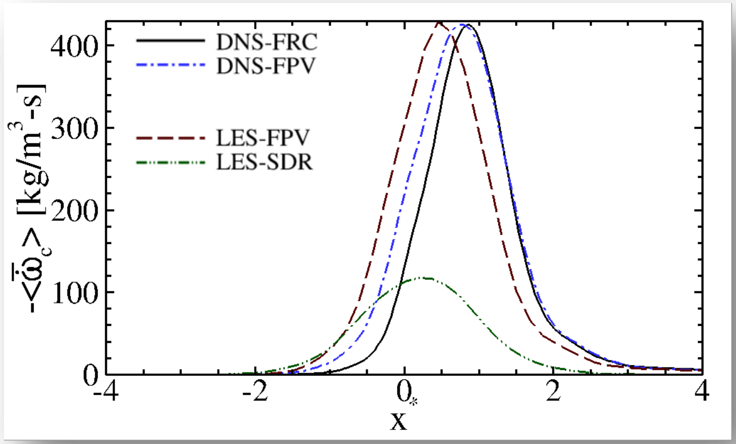
[1]Ma et al., CF 161, (2014), [2]Gao et al., CST 186, (2014)
[3]Ranjan et al., CST 188, (2016)

Statistics of Filtered Reaction Rate

- **Effect of chemistry modeling**
  - DNS-FPV show higher RR in the prog. var. conditional space compared to DNS-FRC
  - Physical space RR can be considered a manifestation of the prog. var. space RR
  - SDR RR not tabulated (unlike FPV)
    - demonstrate wider prog. var. space distributions[1,2] and lower RR magnitudes
- **Effect of turbulence-chemistry modeling**
  - RRLES predictions better than LEMLES[3]



Reaction Rate (RR) in Prog. Var Space

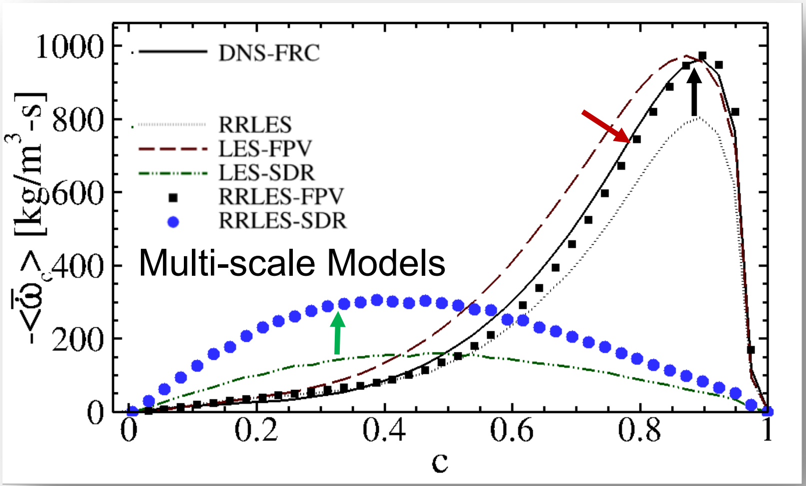


Reaction Rate (RR) in Physical Space

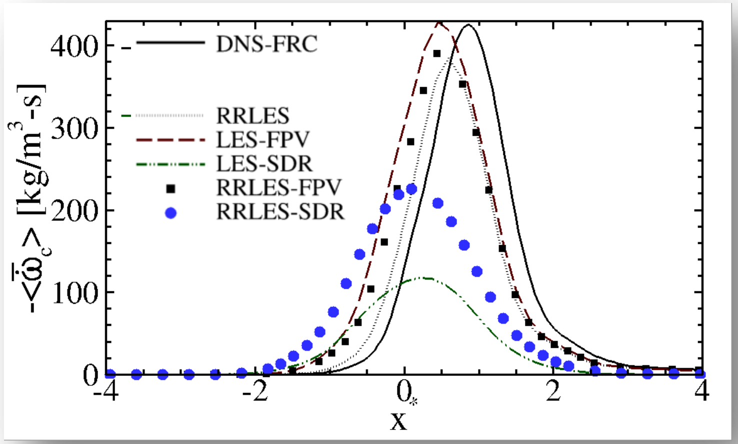
[1]Ma et al., CF 161, (2014), [2]Gao et al., CST 186, (2014)
[3]Ranjan et al., CST 188, (2016)

Statistics of Filtered Reaction Rate

- Effect of chemistry modeling
  - RRLES-FPV show higher RR in the prog. var. conditional space compared to RRLES leading to a closer match to FRC-DNS
  - Physical space RR can be considered a manifestation of the prog. var. space RR
  - SDR RR not tabulated as a function of c (unlike FPV); demonstrate wider prog. var. space distributions[1,2] and lower RR magnitudes
- Effect of turbulence-chemistry modeling
  - RRLES predictions better than LEMLES[3]
  - RRLES-FPV and RRLES-SDR yield better predictions compared to LES-FPV and LES-SDR due to the subgrid LEM modeling



Reaction Rate (RR) in Prog. Var Space

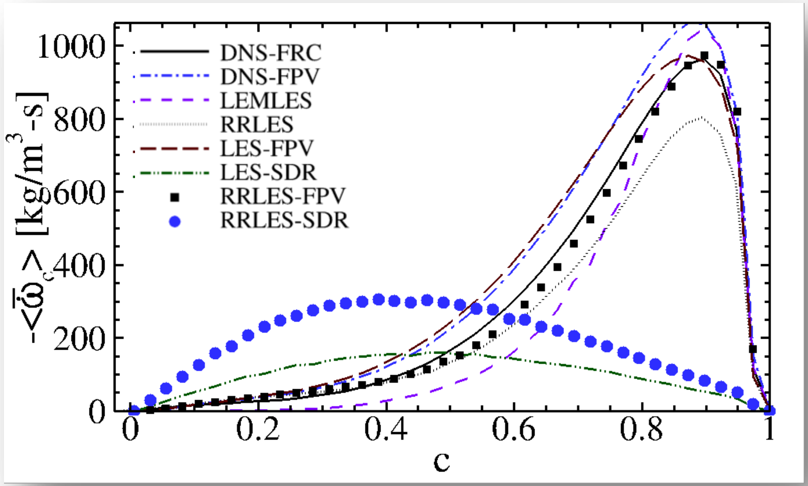


Reaction Rate (RR) in Physical Space

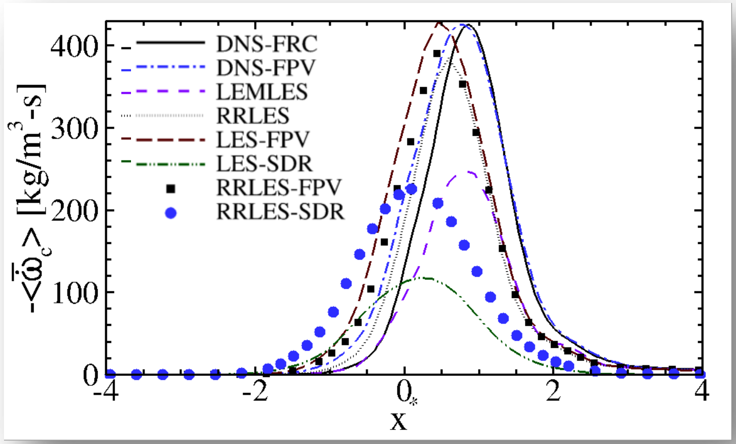
[1]Ma et al., CF 161, (2014), [2]Gao et al., CST 186, (2014)
[3]Ranjan et al., CST 188, (2016)

Statistics of Filtered Reaction Rate

- **Effect of chemistry modeling**
  - DNS-FPV and RRLES-FPV show higher RR in the prog. var. conditional space compared to their FRC variants DNS-FRC and RRLES
  - Physical space RR can be considered a manifestation of the prog. var. space RR
  - SDR RR not tabulated as a function of c (unlike FPV); demonstrate wider prog. var. space distributions[1,2] and lower RR magnitudes
- **Effect of turbulence-chemistry modeling**
  - RRLES predictions better than LEMLES
  - RRLES-FPV and RRLES-SDR yield better predictions compared to LES-FPV and LES-SDR due to the subgrid LEM modeling



Reaction Rate (RR) in Prog. Var Space



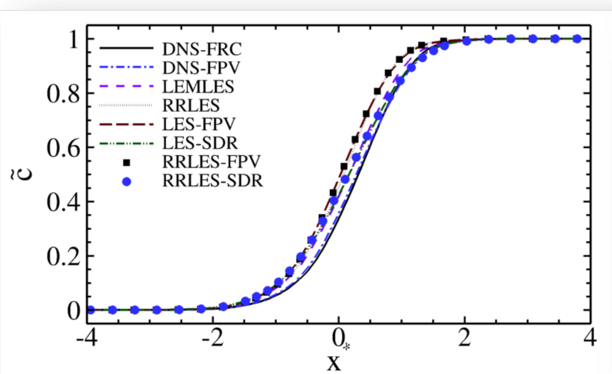
Reaction Rate (RR) in Physical Space

[1]Ma et al., CF 161, (2014), [2]Gao et al., CST 186, (2014)
[3]Ranjan et al., CST 188, (2016)

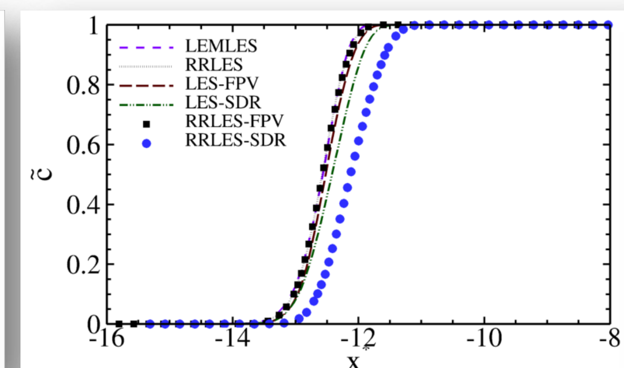
Average Flame Structure

- Average flame structure in physical space captured consistently with all models at different pressures
- Effect of chemistry modeling (FPV vs FRC) in preheat and flame regions in terms of differences in gradient tend to reduce with increase in pressure: **role of small-scale turbulence decreases**
- Major difference observed with SDR closure, which is related to differences in prediction of filtered source term across flame brush: **difference increases with increase in pressure**

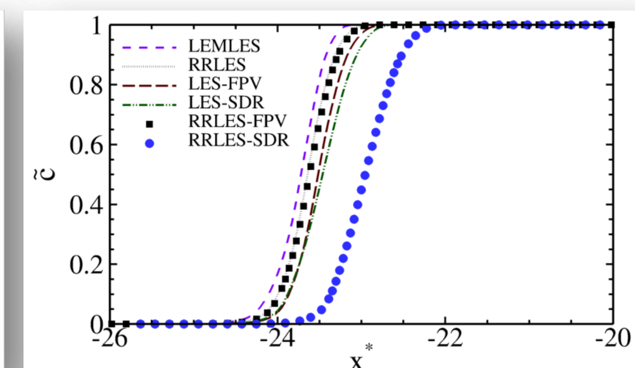
Progress variable variation in physical space



1 atm



5 atm

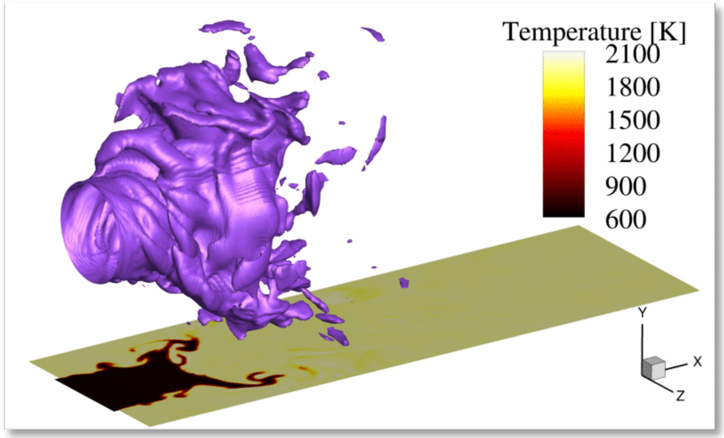


10 atm

Premixed Flame Turbulence: Summary

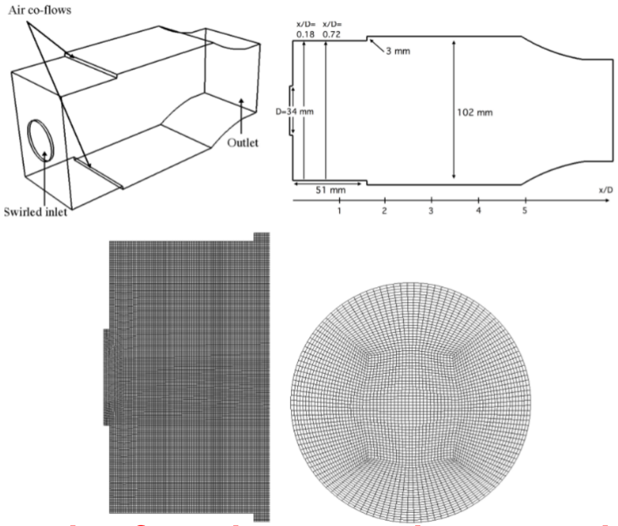
- RRLES allows any reaction rate closure to be included in the subgrid
- FPV/SDR based approaches are cost effective alternatives to FRC
- Qualitatively, all approaches reasonably capture flame features, but quantitative differences are also observed
- Further studies underway including the more recent SDR models
- Methodology is generic and hence can be used for more complex problems

Application to Model Combustor



LEMLES of Combustors: GE LM6000

- premixed swirl combustor
  - Inlet T = 644 K, P = 6 bar, $\phi = 0.6$
  - Flame corresponds to TRZ regime
- Computational grid
  - 524 blocks., 2.2 M grid points
  - Resolution: 0.2-0.6 mm
- Adiabatic temperature/no-slip walls and Char inflow/outflow BC
- Chemistry: 13-species and 73-step[1]
- LEMLES with experiments where co-flow is cold done earlier
- Models assessed by comparing with LEMLES results with hot co-flow of equilibrium products



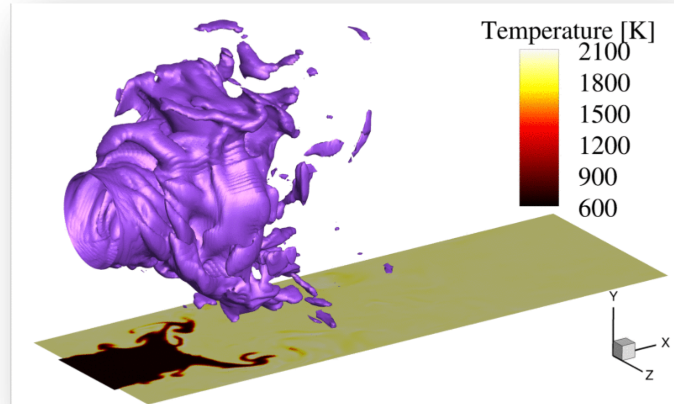
Schematic of combustor and computational grid

Case	CPU Hrs for a flow through time (Relative Speedup)
QLLES	971 **(2.22)**
LEMLES	5580 **(0.85)**
RRLES	4270 **(1.00)**
FPV-LES	971 **(4.86)**
SDR-LES	858 **(5.50)**
FPV-RRLES	1890 **(2.50)**
SDR-RRLES	2120 **(2.23)**

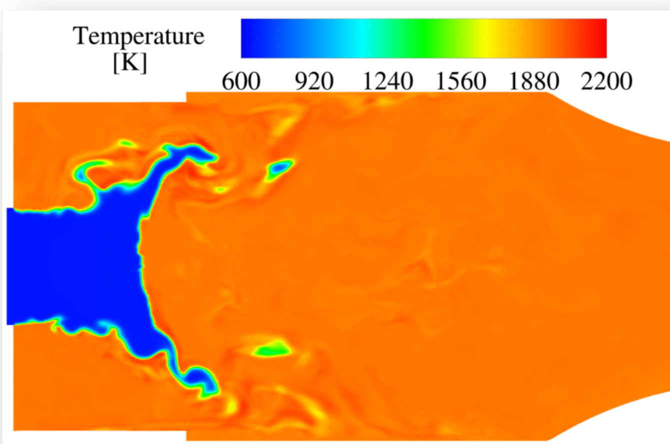
[1] *Sankaran et al. (2007)*

Reacting Flow Features

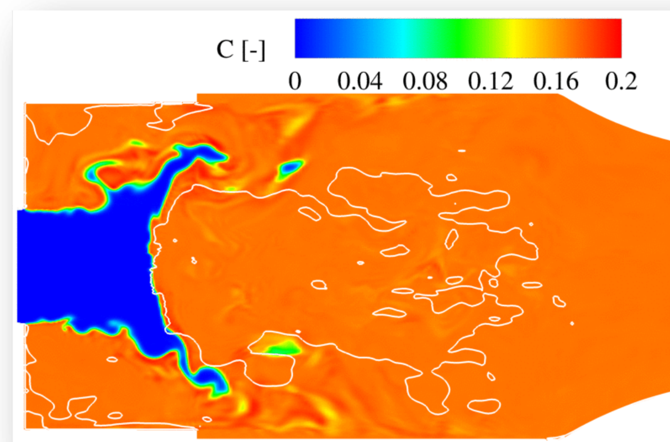
- Flame holding occurs in shear-layers due to swirling flow, which creates vortex breakdown bubble (VBB)
- Highly unsteady behavior of VBB observed
- Interaction of shear layers occurs with co-flow
- Progress variable field appears to be correlated with temperature field



Temperature iso-surface (1800 K) with contours on central plane



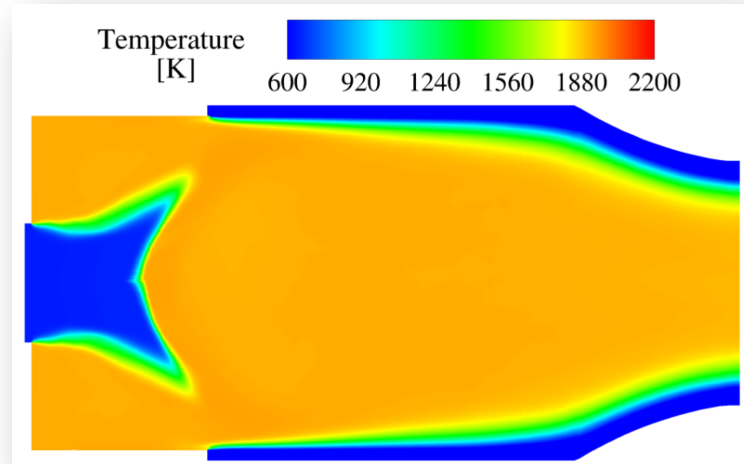
Temperature



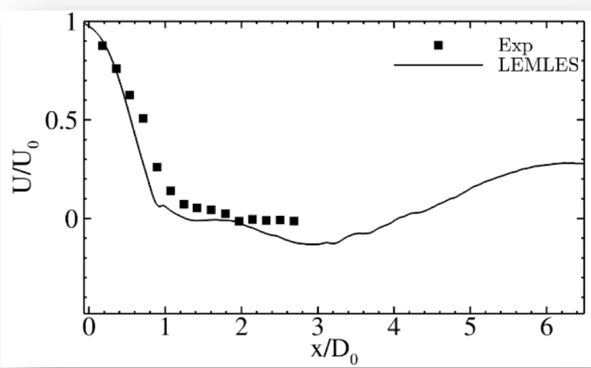
Progress variable overlaid with zero axial velocity curves

Validation Study

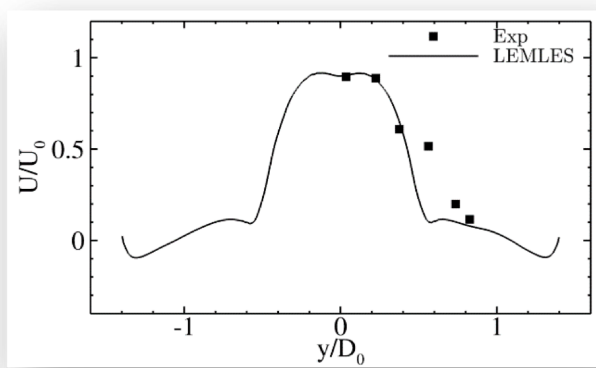
- Co-flow is set to cold conditions in order to match the experiments
- LEMLES serve as reference for assessment of other models



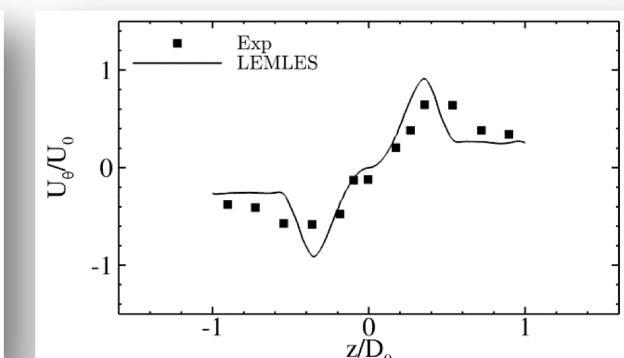
Mean temperature in central plane



Axial centerline velocity



Axial velocity at x/D_0 = 0.18

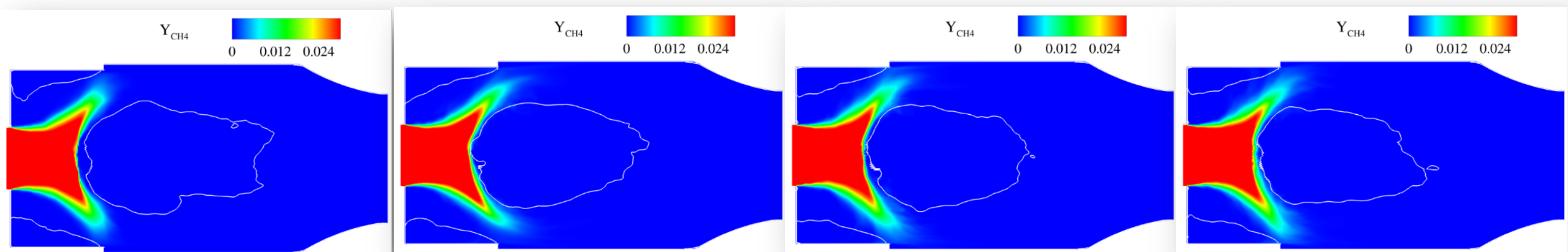


Tangential Velocity at x/D_0 = 0.18

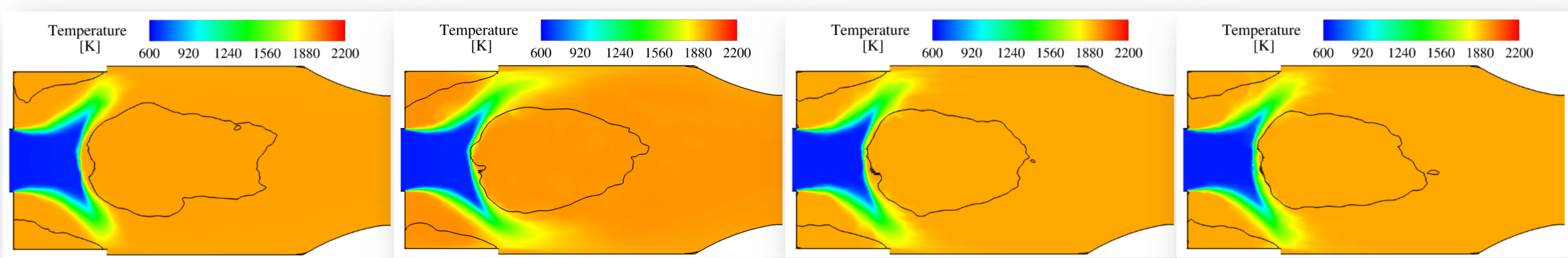
Effect of Turbulent Combustion Modeling

- Overall very similar flame and VBB observed for all models
- Co-flow needs to be burnt solution for these studies
- LES-SDR and RRLES-SDR still being evaluated

LEMLES RRLES LES-FPV RRLES-FPV



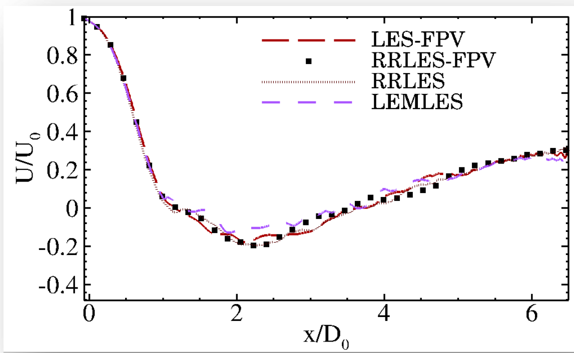
Mean CH_4 mass fraction contour overlaid with zero mean axial velocity curves



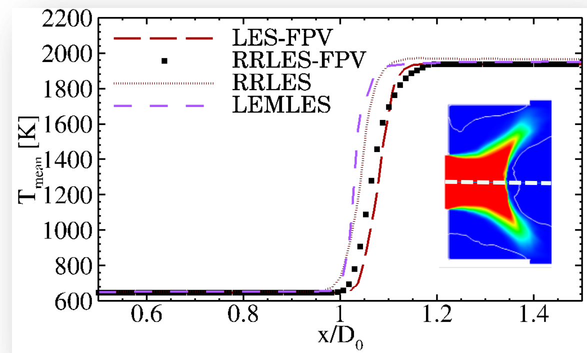
Mean temperature overlaid with zero mean axial velocity curves

Effect of Turbulent Combustion Modeling

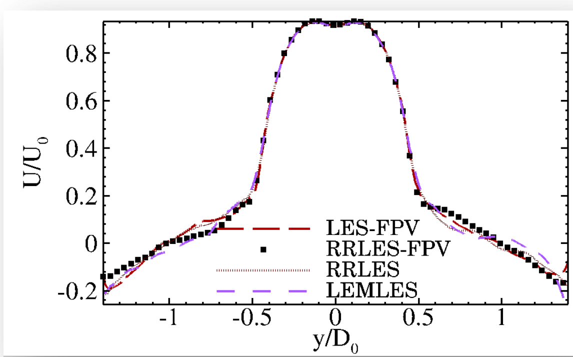
- Axial centerline and VBB not affected by turbulence/chemistry modeling
- Differences in the temperature across the flame visible when zoomed in
  - Behavior similar between LEMLES and RRLES
  - RRLES-FPV closer to RRLES compared to LES-FPV



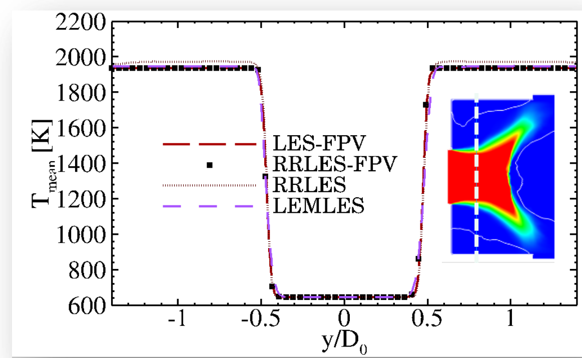
Mean axial centerline velocity



Mean centerline temperature



Mean axial velocity at $x/D_0 = 0.18$



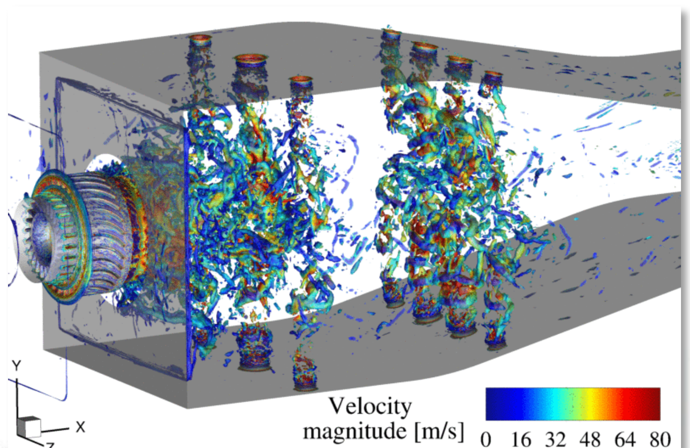
Mean temperature $x/D_0 = 0.18$

GE LM6000 Combustor: Summary

- All modeling approaches give similar results for global quantities such as temperature and axial velocity
  - flame is highly turbulent and close to thin flame assumption
- Differences still exist locally and need further assessment
  - Similar flame structure for LEMLES and RRLES
  - RRLES-FPV closer to RRLES then LES-FPV
- Compressible FPV and SDR models still need to be assessed
- Computations are very fast and all cases doable in matter of hours

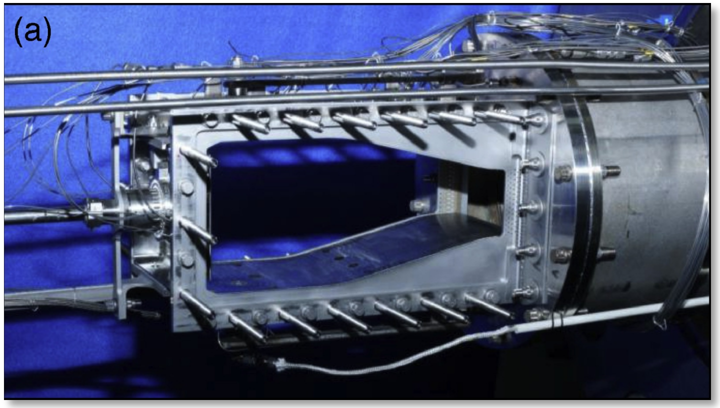
National Jet Fuels Combustion Program

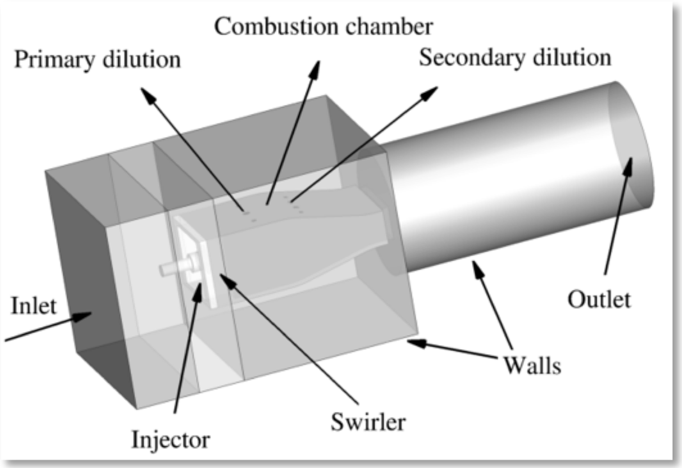
CFD Teams:
Stanford, GaTech,
ANL/Purdue, NASA Glenn



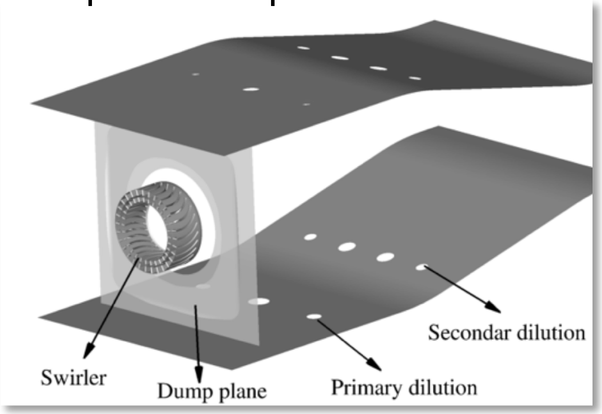
LES of UDRI Rig

- Swirl spray combustor hosted at AFRL, Dayton[1,2]
- Representative of a real gas turbine combustor
  - 3 swirlers, 14 dilution jets, Multiple effusion cooling holes





Complete Computational Domain



Combustor

Inlet Air	391.4 g/s, 394 K
Fuels	Cat A2 (2.55 g/s, 322 K), Cat C1 (2.50 g/s, 322 K)
Pressure	206 kPa
Swirlers	Radial (24 vanes) Inner/outer axial (30 vanes)

[1]L. Esclapez et al., Combust. Flame 181 (2017)
[2]M. Colket et al., AIAA J., 55(4), 2017

Chemistry and Fuel Effects Modeling

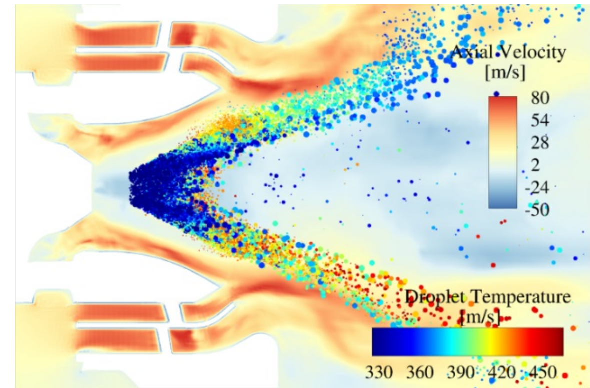
- Real fuels contain thousands of components, impractical to track all
- Reduced HyChem approach with lumped kinetic parameters derived from experiments, and further reduction of the mechanism to a non-stiff variant
- Partially stirred reactor (PaSR) as turbulent combustion closure
- Non-reacting (NR) simulation carried out for initial verification
- A2 (~$C_{11}H_{22}$) – conventional jet fuel, C1 (~$C_{13}H_{28}$) – alternate jet fuel
- Reacting simulations are very costly due to large number of species and reaction steps (**~ 2 months on 2100 processors**)
- 21 million structured cells for the entire test rig

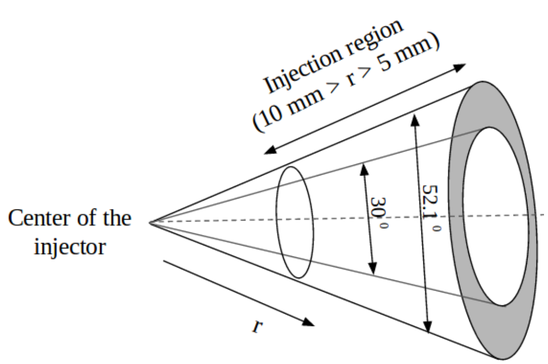
Case Name	Fuel	Equivalence Ratio	CPU-Hours for one flow-through (20 ms)	Number Species	Number Steps
NR	-	Non-reacting	**0.04 million**	-	-
A2 $^{0.096}$	A2	0.096 (NBO)	**0.80 million (20 x NR)**	31	202
C1 $^{0.096}$	C1	0.096 (NBO)	**0.64 million (16 x NR)**	27	182

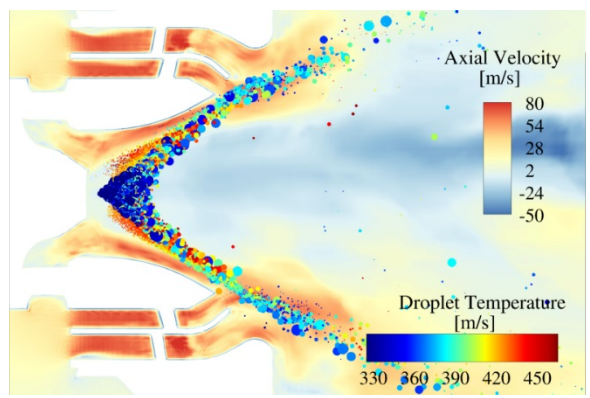
[1]Wang et al. Combust. Flame, 2018; [2]Gao Y., Lu T. private communication, 2017, [3]Sankaran et al., AIAA-2016-1449

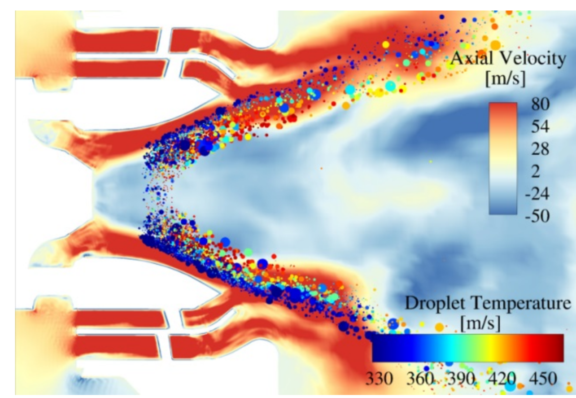
Sensitivity to Spray Injection

- **Injection A:** Narrow truncated hollow cone
- **Injection B:** Wide truncated hollow cone
- **Injection C:** Hollow cone
- Dense spray conditions are unknown
- Dilute distribution defined based on downstream measurements but initial development unknown
- Can this be sufficient to predict LBO?



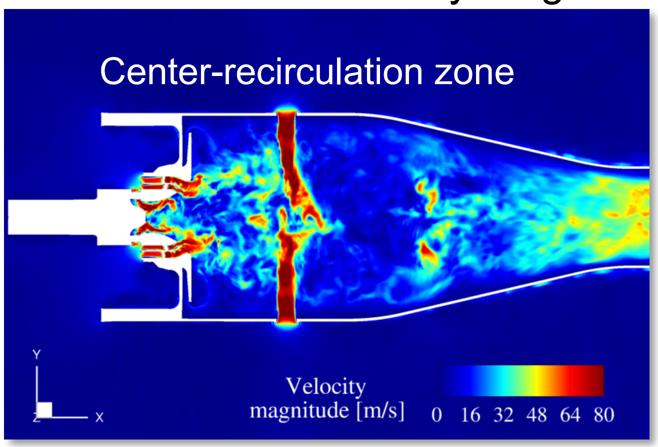




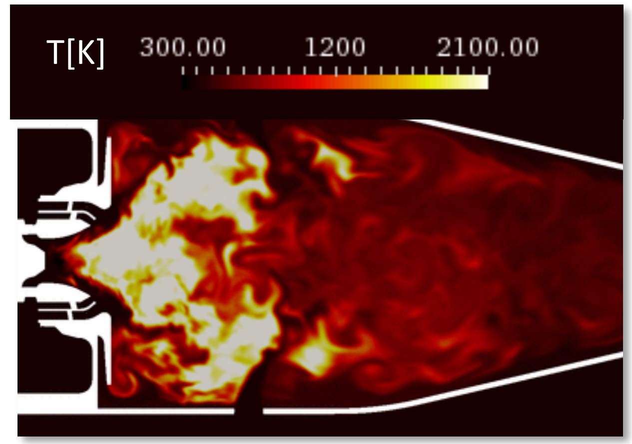


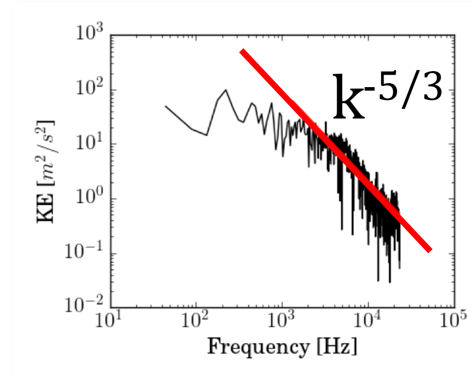
Flow/Flame Features

Center-slice: velocity mag.

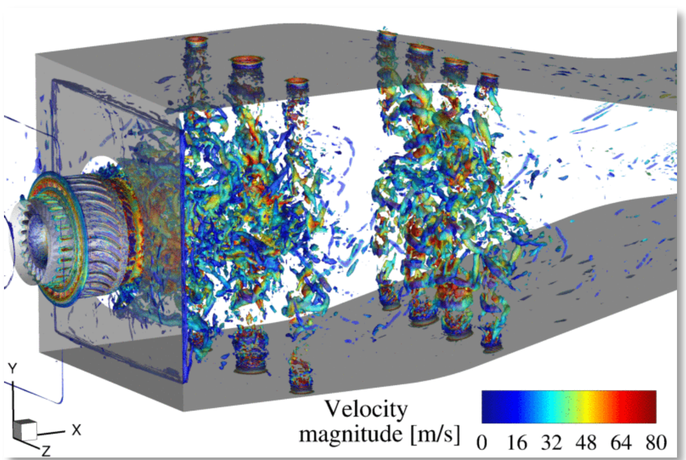


Center-slice: Temperature

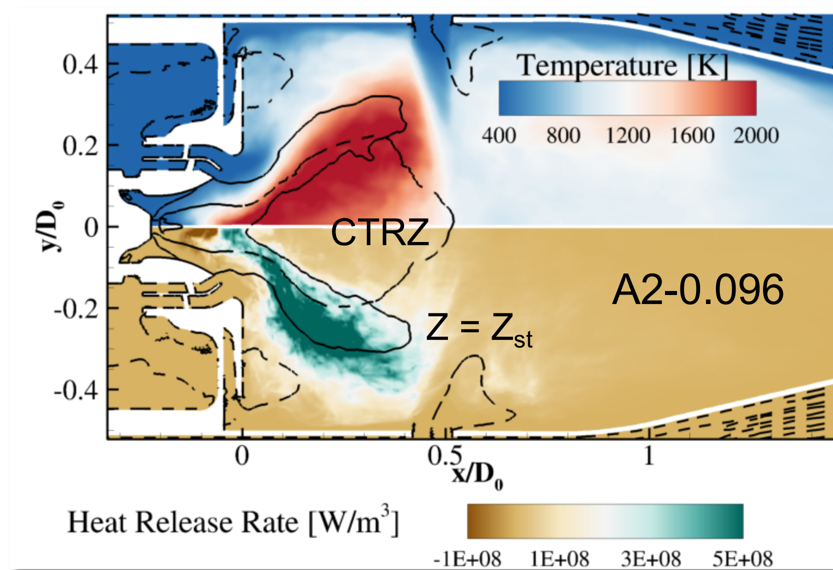




KE spectra in shear layer



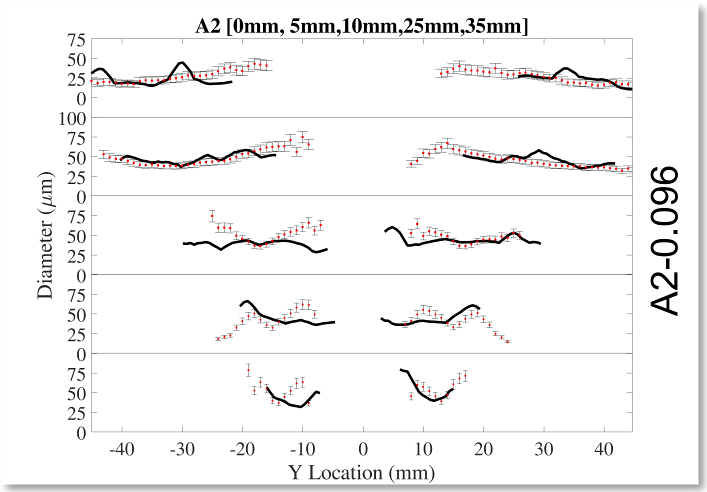
Combustion Chamber: Q-Criterions



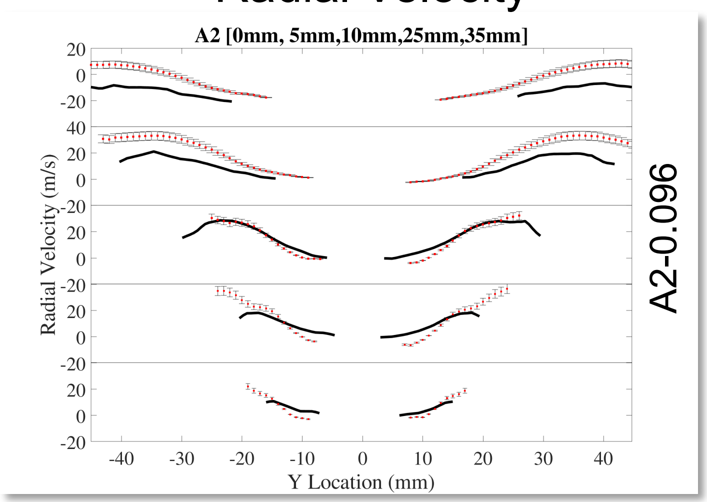
Time-Averaged Center-slice contours

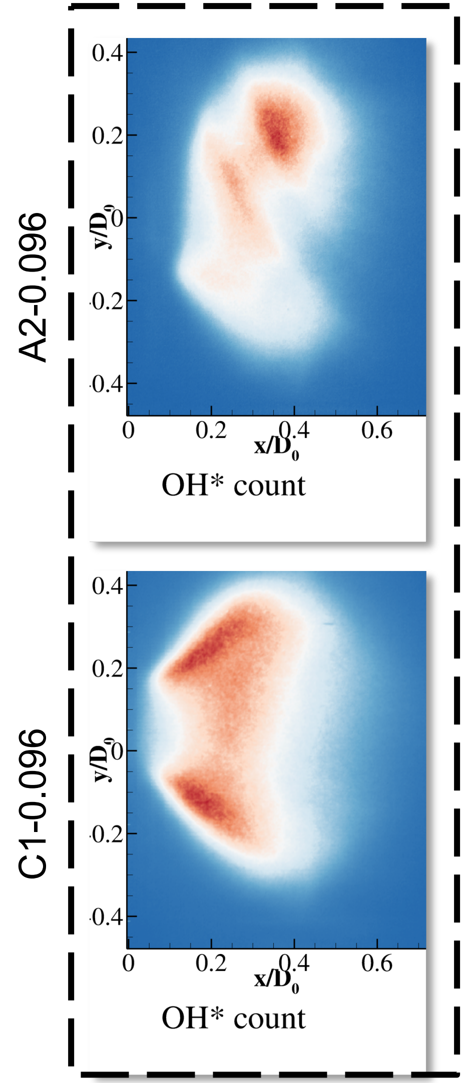
Validation Against Experimental Data

Sauter Mean Diameter

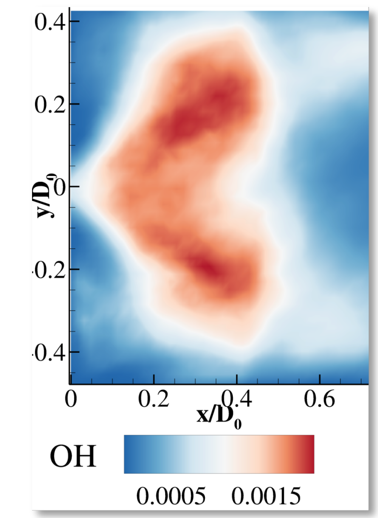


Radial Velocity





Expt. OH PLIF

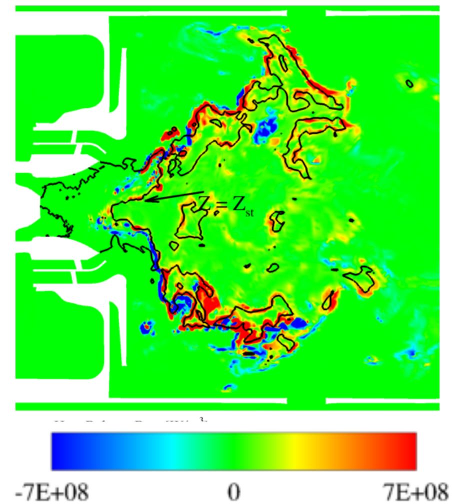


LES Line-of-Sight

[1]Panchal et al., AIAA JPC, AIAA-2018-4684, 2018

Challenges and Ongoing Work

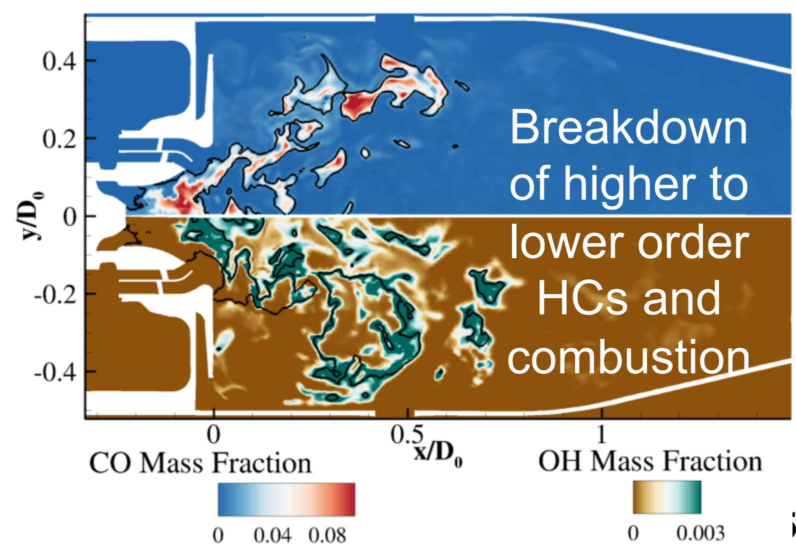
- Partially premixed burning
- Complex effects of FRC
  - Pyrolysis process
  - Localized extinctions
  - auto-ignitions
- Finite-rate computational cost very high – even more with LEMLES/RRLES
- Transient effects need a long time to settle down
- Goal is to predict LBO due to fuel chemistry effects
  - Still not achieved!!



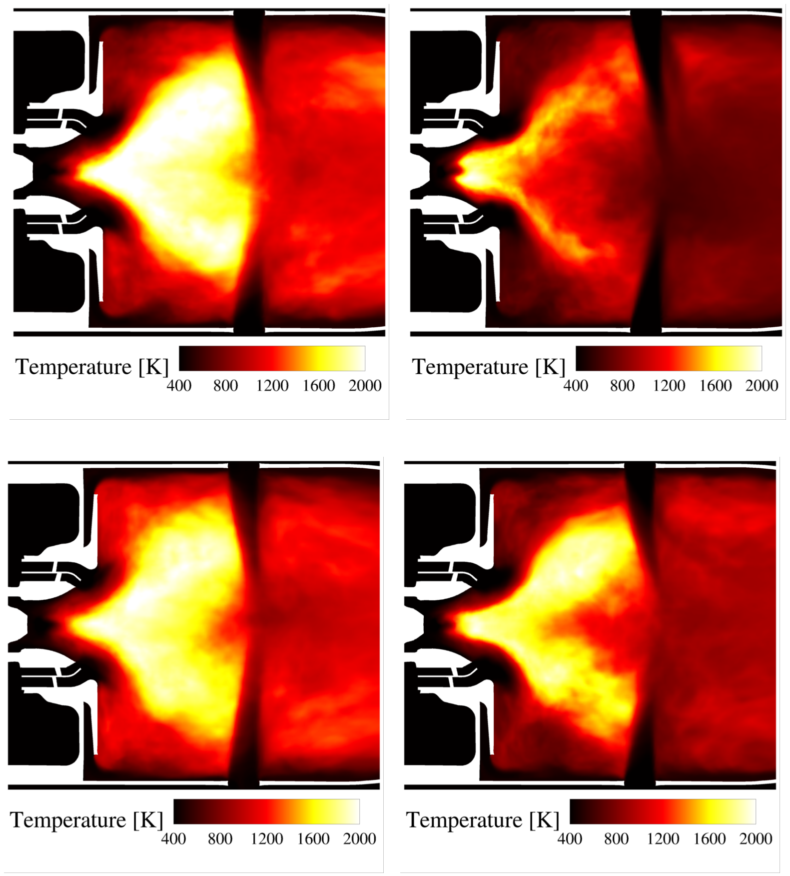
Takeno Flame Index: Partially Premixed Burning

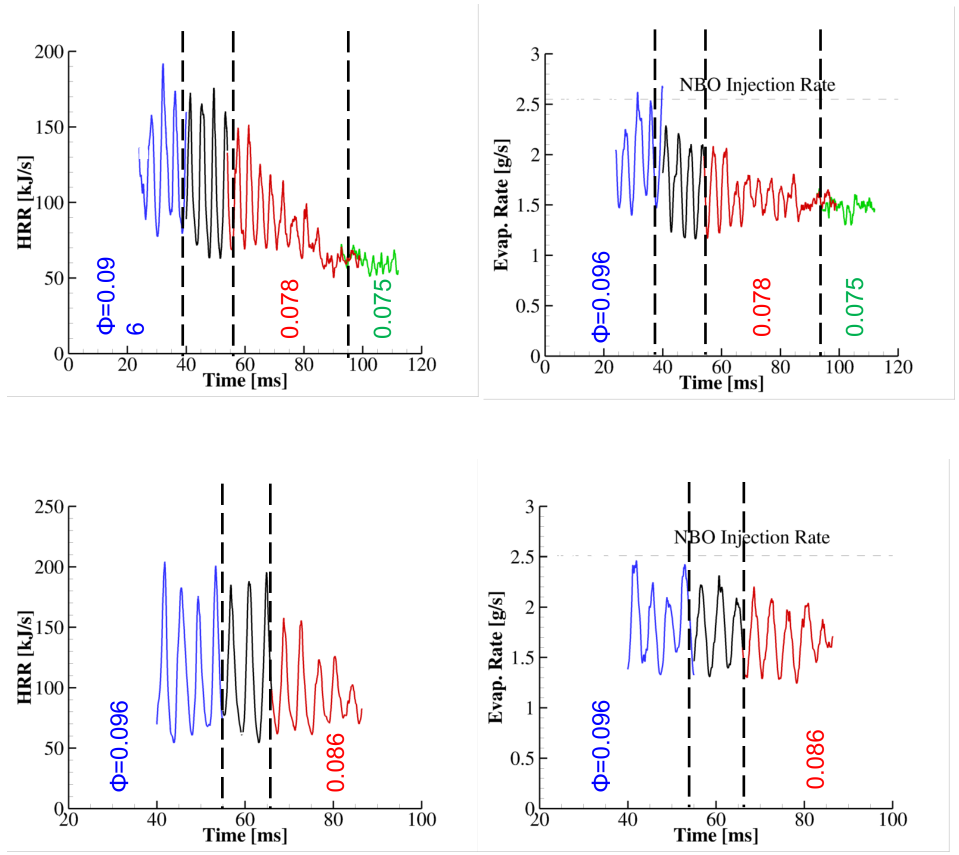
A2-0.096

Premixed Non-Premixed



GTech LBO simulation still unresolved





Future Prospects?

- Many challenges for real engine relevant transient problems
  - CI, LBO, cold start, altitude restart are some key challenges for design
  - Realistic configurations have many uncertainties in BC and IC that experimental studies cannot isolate or define
    - Computational tools can be used to assess but can lead to many dead ends
  - Brute force simulations are expensive but doable but huge dataset
    - Need big data tools and co-processing to analyze on-the-fly
  - Simplified models (e.g., FPV/SDR) may work for some applications but need reliable co-effective methods for spray partially premixed systems
  - Spray BCs are nearly impossible to