# Turbulent Counterflow Flames (TCF): Modeling and Simulation


*Coordinators:*

**Bruno Coriton**

**Steve Pope**


**Twelfth International Workshop on Measurement and Computation of Turbulent Flames (TNF12)**

**July 31st – August 2nd, 2014**

**Pleasanton, CA**

# TNF12: TCF Modeling and Simulation Contributions

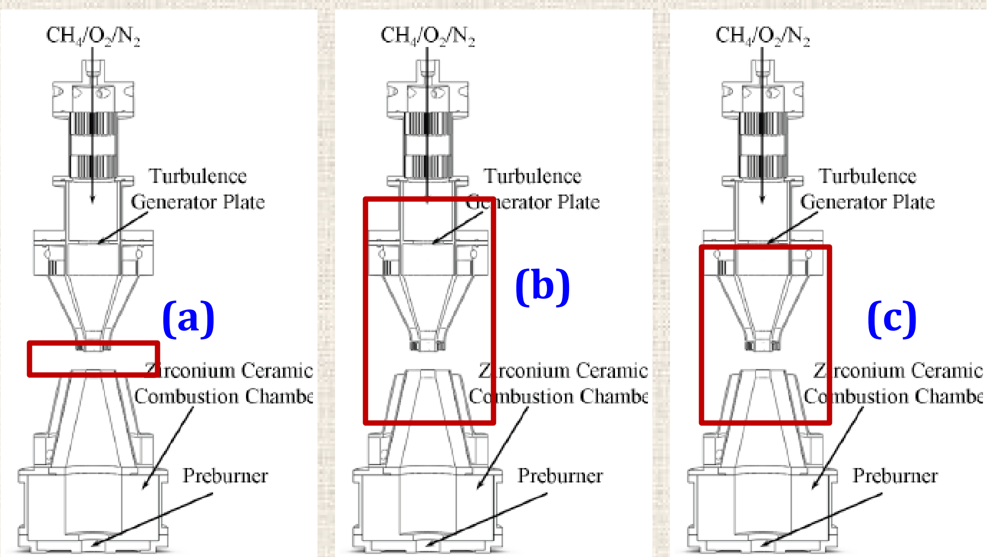
| Name | Institutions | Researchers | Method |
|---|---|---|---|
| Brandenburg | Brandenburg Technical University | Z. Jozefik, A. R. Kerstein, H. Schmidt | ODT |
| CRAFT Tech. | CRAFT Tech. | K. Kemenov, W. Calhoon, Jr. | LES/c |
| Duisburg-Essen | University of Duisburg-Essen, UC Berkeley, Imperial College | M. Rieth, F. Proch, A. Kempf, J.-Y. Chen, P. Lindstedt | LES/FDF |
| Cornell | Cornell University, Sandia, Yale | R. Tirunagari, S. B. Pope, B. Coriton, A. Gomez, J. H. Frank | LES/PDF |

# Previous Published Simulations

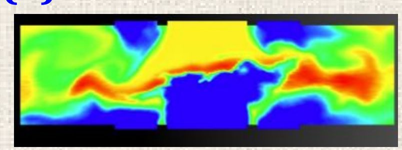

- Pettit, M.W.A., Coriton, B., Gomez, A., and Kempf, A.M., "Large-Eddy Simulation and Experiments on Non-premixed Highly Turbulent Opposed Jet Flows," Proceedings of the Combustion Institute, 33 (2011), 1391-1399
- Kim, I.S., Mastorakos, E., “Simulations of Turbulent Non-premixed Counterflow Flames with First-order Conditional Moment Closure,” Flow Turbulence and Combustion, 76 (2006), 133-162
- Geyer, D, Kempf, A, Dreizler, A, Janicka, J., “Turbulent Opposed-jet Flames: A Critical Benchmark Experiment for Combustion LES”, Combustion and Flame, 143 (2005), 524-548
- Geyer, D., Dreizler, A., Janicka, J., Permana, A.D., and Chen, J.Y., “Finite-rate Chemistry Effects in Turbulent Opposed Flows: Comparison of Raman/Rayleigh Measurements and Monte Carlo PDF Simulations,” Proceedings of the Combustion Institute, 30 (2005), 711-718
- Kempf, A., Forkel, H., Sadiki, A., Janicka, J., and Chen, J.-Y., “Large Eddy Simulation of a Counterflow Configuration with and without Combustion,” Proceedings of the Combustion Institute, 28 (2000), 35-40
- Erkstein, J., Chen, J.Y., Chou, C.P., and Janicka, J., “Modeling of Turbulent Mixing in Opposed Jet Configuration: One-Dimensional Monte Carlo Probability Density Function Simulation,” Proceedings of the Combustion Institute, 28 (2000), 141-148

# Major Issue: Solution Domain and Inflow Velocity Boundary Conditions

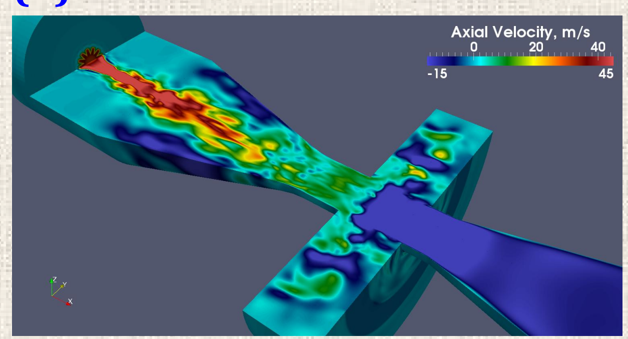
| Group | Domain boundaries | Inflow 1 | Inflow 2 | Cells | Part. |
|---|---|---|---|---|---|
| Brandenburg | a) Nozzle exit planes | Passot-Pouquet spectrum | Laminar | - | - |
| CRAFT Tech. | b) Upstream of TGP | Uniform | Uniform | 1.7/6m | - |
| Duisburg-Essen | a) and c) Downstream planes of TGPs | Uniform | Uniform | 1.7m | 6m |
| Cornell | a) Nozzle exit planes | Scaled LES data | Laminar | 0.3m | 6m |




(a)



(b)




(c)

# Flames Studied

| Group | Target | Configuration | Stream 1 | Stream 2 |
|---|---|---|---|---|
| Brandenburg | Sandia DNS | Premixed/Burnt | $H_2$/air, φ=0.4, 294K | $H_2$/air, φ=1.0, 1475K |
| CRAFT Tech. 1 | Sandia/Yale | Inert/Burnt | $N_2$, 294K | $CH_4/O_2/N_2$, φ=1.0, 1850K ($O_2/N_2$: 26/74 % mole) |
| CRAFT Tech. 2 | Sandia/Yale | Premixed/Burnt | $CH_4/O_2/N_2$, φ=0.85, 294K ($O_2/N_2$: 30/70 % mole) | $CH_4/O_2/N_2$, φ=1.0, 1850K ($O_2/N_2$: 26/74 % mole) |
| Duisburg-Essen 1 | Darmstadt | Fuel/Air | $CH_4$/air, φ=2.0, 300K | Air, 300K |
| Duisburg-Essen 2 | Imperial College | Premixed/Premixed | $CH_4$/air, φ=0.9, 300K | $CH_4$/air, φ=0.9, 300K |
| Cornell 1 | Sandia/Yale | Inert/Inert (cold) | $N_2$, 294K | $N_2$, 294K |
| Cornell 2 | Sandia/Yale | Fuel/Oxidant | $CH_4/N_2$, 294K (35/65 % mole) | $O_2$, 294K |
| Cornell 3 | Sandia/Yale | Inert/Burnt | $N_2$, 294K | $CH_4/O_2/N_2$, φ=1.0, 1850K ($O_2/N_2$: 26/74 % mole) |
| Cornell 4 | Sandia/Yale | Premixed/Burnt | $CH_4/O_2/N_2$, φ=0.85, 294K ($O_2/N_2$: 30/70 % mole) | $CH_4/O_2/N_2$, φ=1.0, 1850K ($O_2/N_2$: 26/74 % mole) |

# BRANDENBURG

## ODT Modeling of a Counterflow Flame Under Intense Turbulence and Strain with Comparison to DNS

Z. Jozefik[1], A. R. Kerstein[2], and H. Schmidt[1]

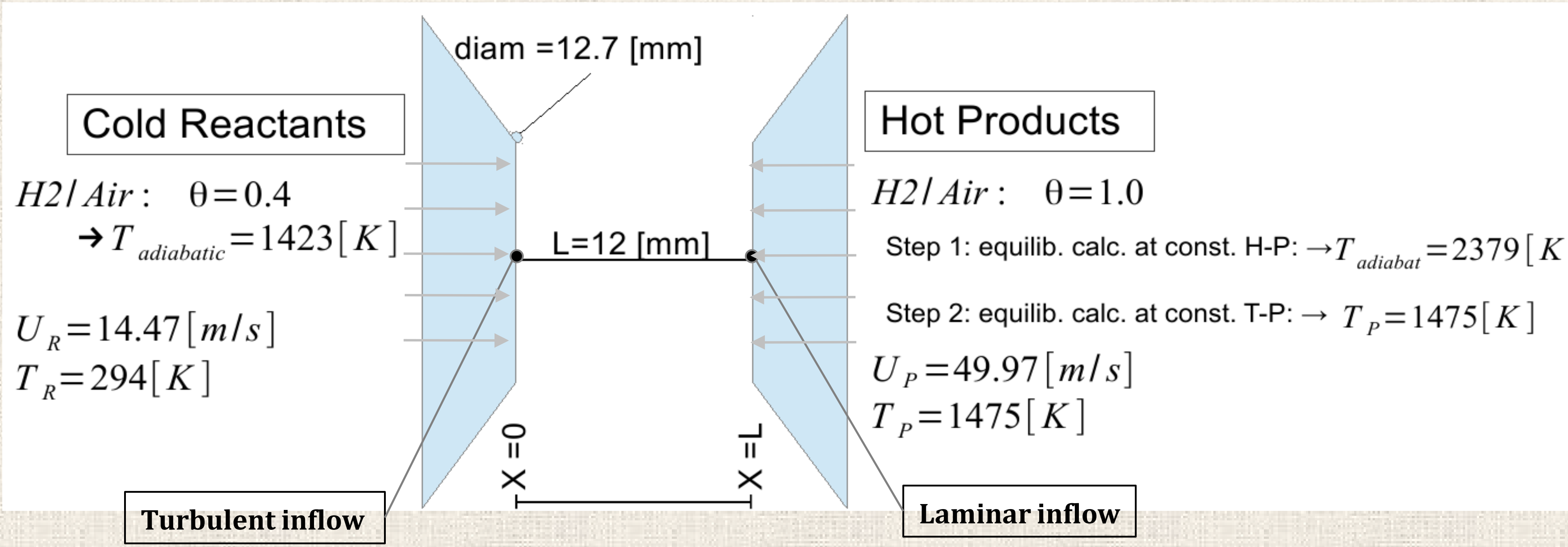
[1]Brandenburg Technical University Cottbus-Senftenberg, Germany
[2]Consultant, Danville, CA. USA

## DNS results by

S. Lyra[3], H. Kolla[3], and J. H. Chen[3]

[3]Combustion Research Facility, Sandia National Laboratories, Livermore, CA. USA

# Configuration




## Flow field characteristics:

- **bulk strain rate:** $a = 2U_R / L = 2{,}400\ s^{-1}$ ; **residence time:** $\tau_R = 0.5L / U_R = 0.4\ ms$

## Reactant stream turbulent inlet conditions:

- **Velocity fluctuations based on a Passot-Pouquet energy spectrum are superimposed on the mean inlet vel.**

- **Characteristic values are:** $L' = 3.6\ mm$, $u' = 5.1\ m/s$

# Model (See Poster for Details)

**Formulation:**

- ODT – one-dimensional turbulence
- 1D
- Lagrangian formulation
- Variable density zero-Mach-number equations

**Empirical Input:**

- ODT viscous penalty parameter Z
- ODT eddy frequency parameter C
- Maximum eddy size allowed is 5 mm= 1.4 *L'*
- Stagnation point location for advection model

**Turbulence:**

- In ODT, turbulent motions that accelerate mixing are modeled through a series of stochastic rearrangement events
- Each event interrupts the system evolution, applying an instantaneous transformation to the property fields over some spatial interval

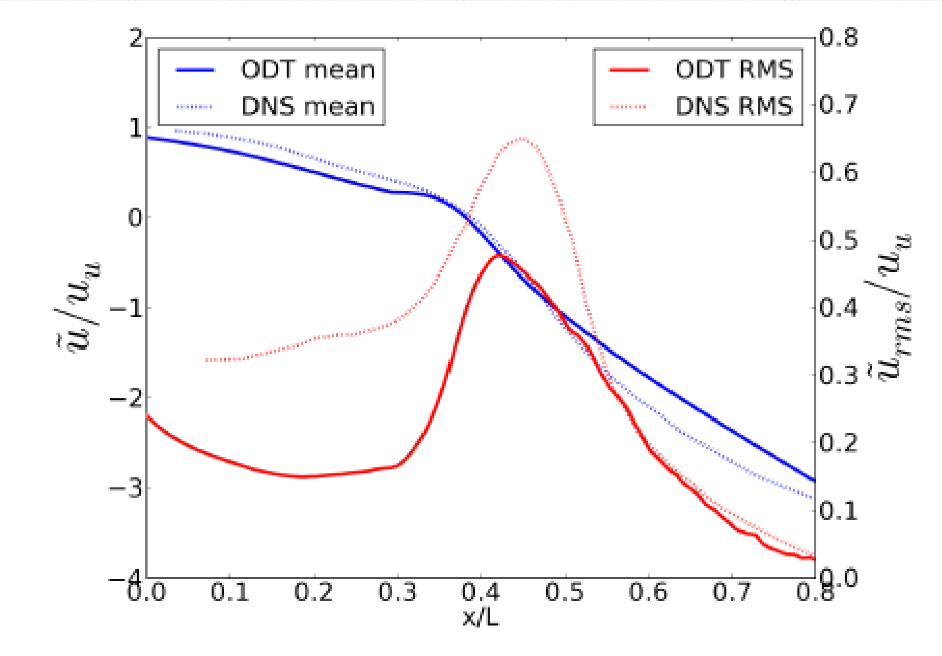
**Chemistry:**

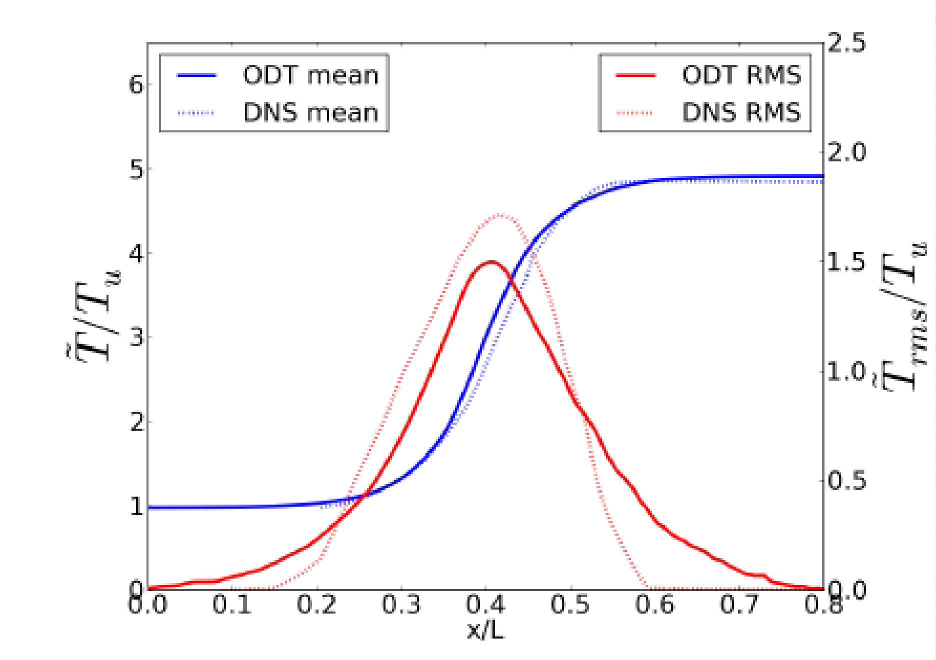
- Thermodynamic properties and reaction rates are calculated using CANTERA

**Numerics:**

- Adaptive grid
- Equations are solved using standard 2nd-order finite-difference discretization
- Time integration is performed using the CVODE code of SUNDIALS

# Results: Favre Averaged Mean and RMS Profiles of Velocity and Temperature



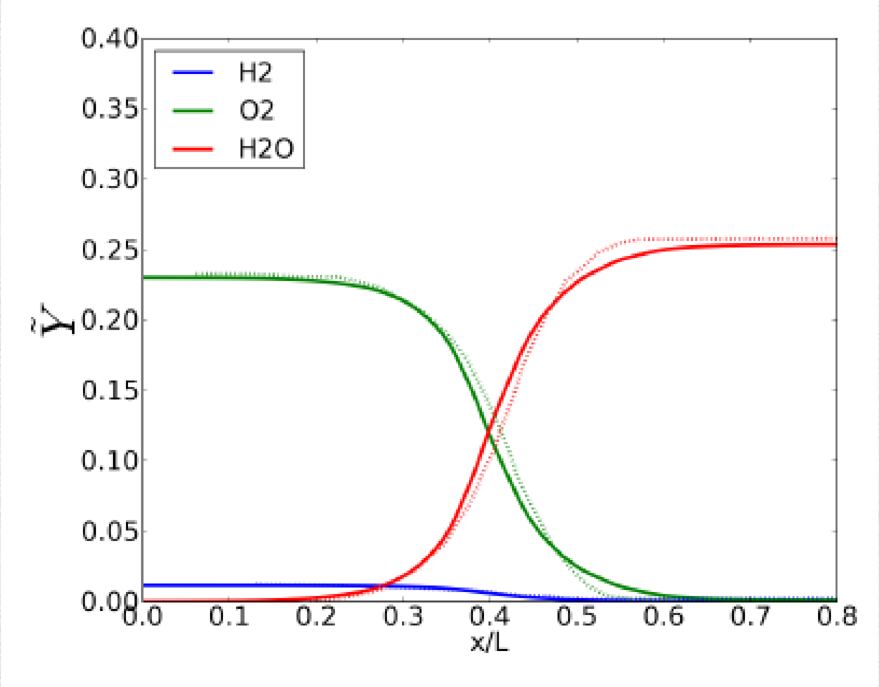



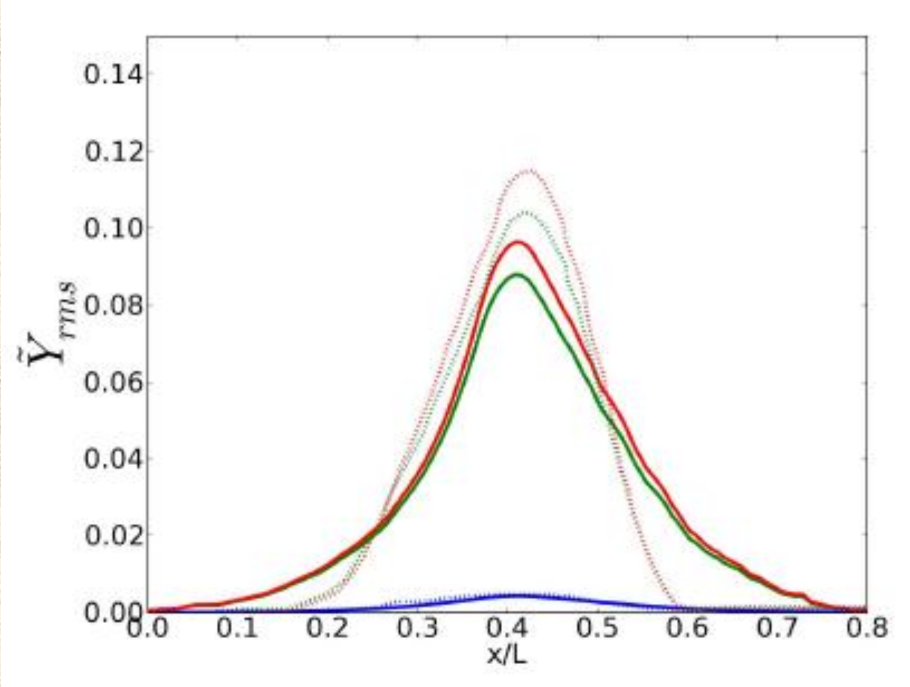

1) Good overall comparison to DNS data is achieved

2) Mean velocity is in good agreement near stagation point. Away from stagation point, our linear advection model underestimates DNS

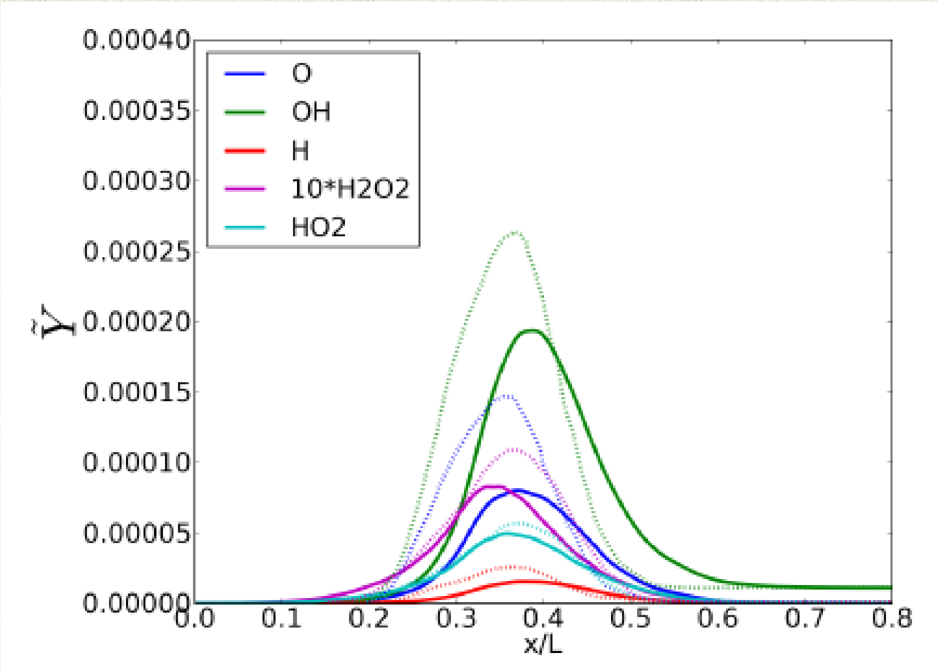
3) RMS profiles are underpredicted, due to the velocity being slowed down too much. As a result, not enough turbulence is generated around the stagation point

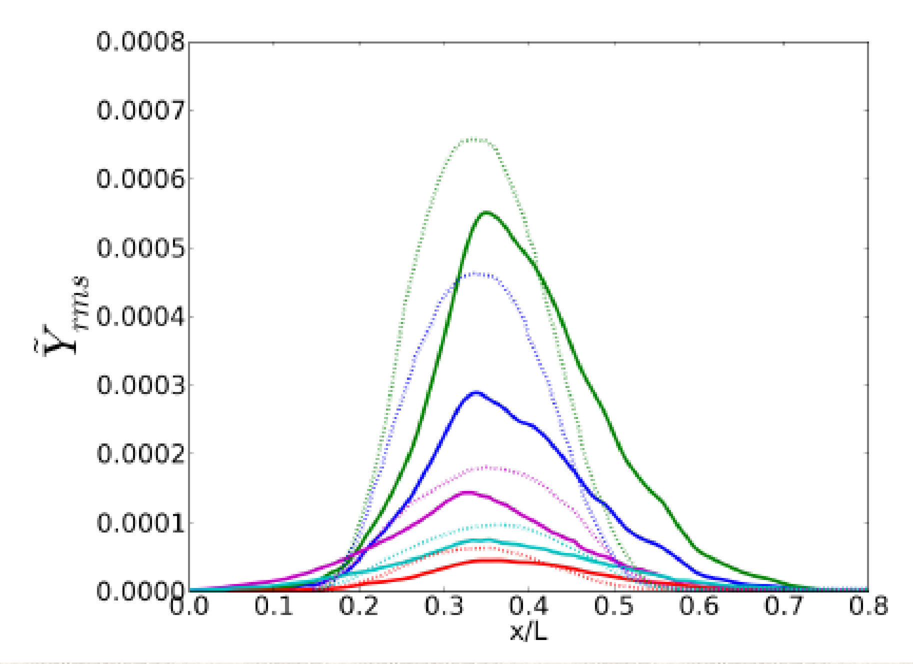
# Results: Favre Averaged Mean and RMS Profiles of Major Species



# Results: Favre Averaged Mean and RMS Profiles of Minor Species



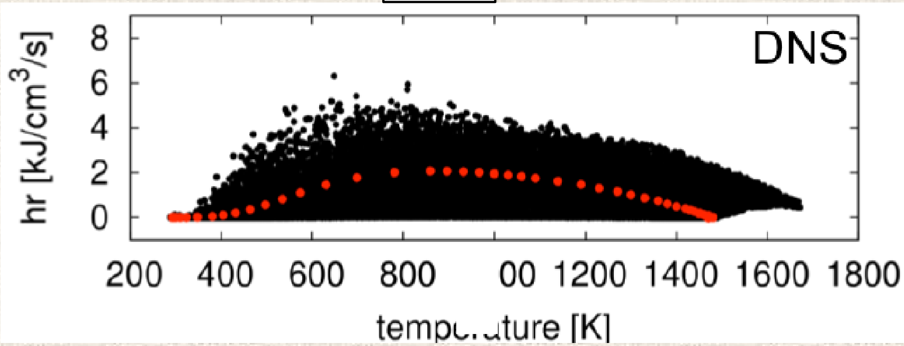



# Results: Scatter Plots

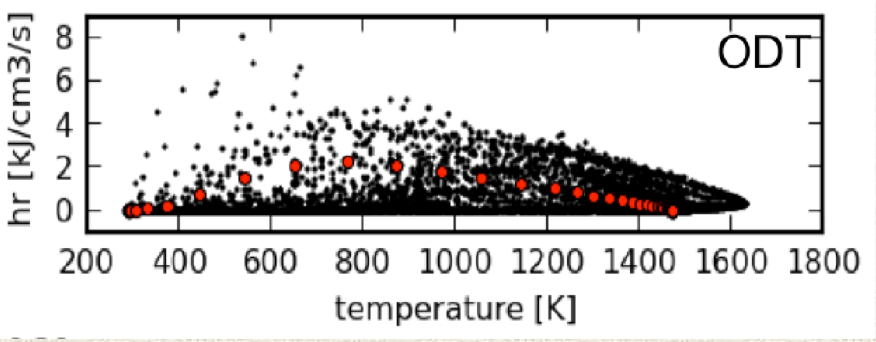
**Legend:**
● = strained laminar flame
$strain = 2U_R / L = 2{,}400\ s^{-1}$

## Heat release rate

**DNS**

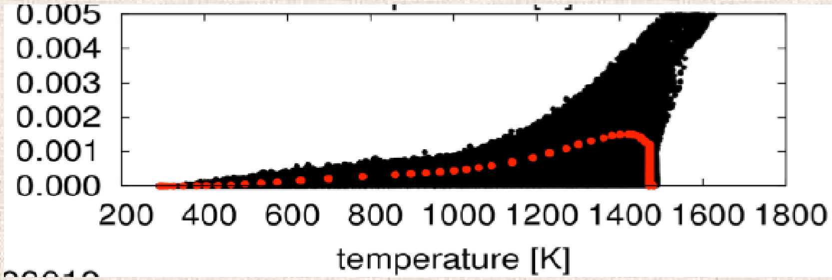



**ODT**

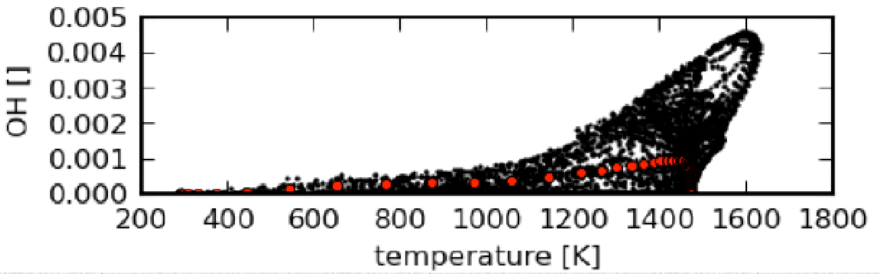



## Minor species OH

**DNS**

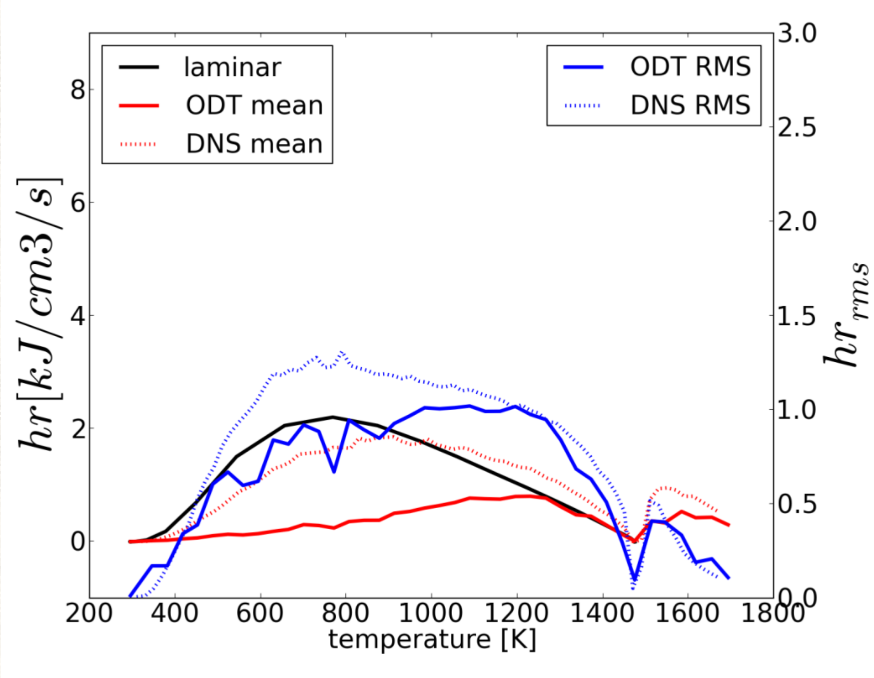


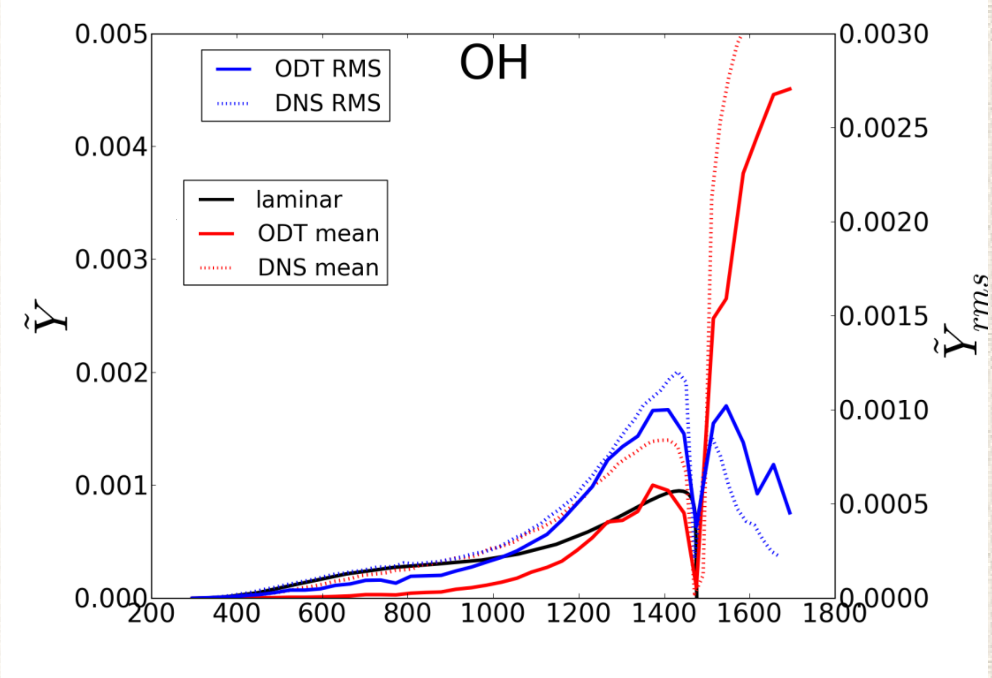

**ODT**




**1) ODT is able to capture the range of results shown by DNS.**

# Results: Statistics Conditioned on Temperature



# BRANDENBURG: Conclusions

- Although ODT is a reduced order model, it is able to achieve overall good agreement with DNS

- Mean temperature, major species, and some minor species show: quantitative agreement with DNS

- Scatter plots show: range of DNS results is captured by ODT

- Conditional statistics for heat release rate show: ODT underpredicts ignition

- The methane/air reactant-to-product experiment was also attempted with ODT:
  - Here, our model does not capture the level of re-ignition shown in the experiment.
  - We believe, that for the exp., advection from off the center line has a major role on ignition detected on the line.
  - Comparing the DNS to the exp. setup:
    - a) the exp. axial range is larger, 16 mm vs 12 mm for the DNS
    - b) the exp. reactant stream bulk inlet velocity is slower, 11.2 m/s vs 14.49 m/s for the DNS
    - c) for the exp., the product stream temp. is below the adiabatic flame temp. of the reactant stream mixture, while for the DNS it is above.

## Future Work:

- ODT vs DNS:
  - Run further comparisons to identify cause of underignition.

- ODT vs EXP.:
  - Learn from/ compare to LES results.

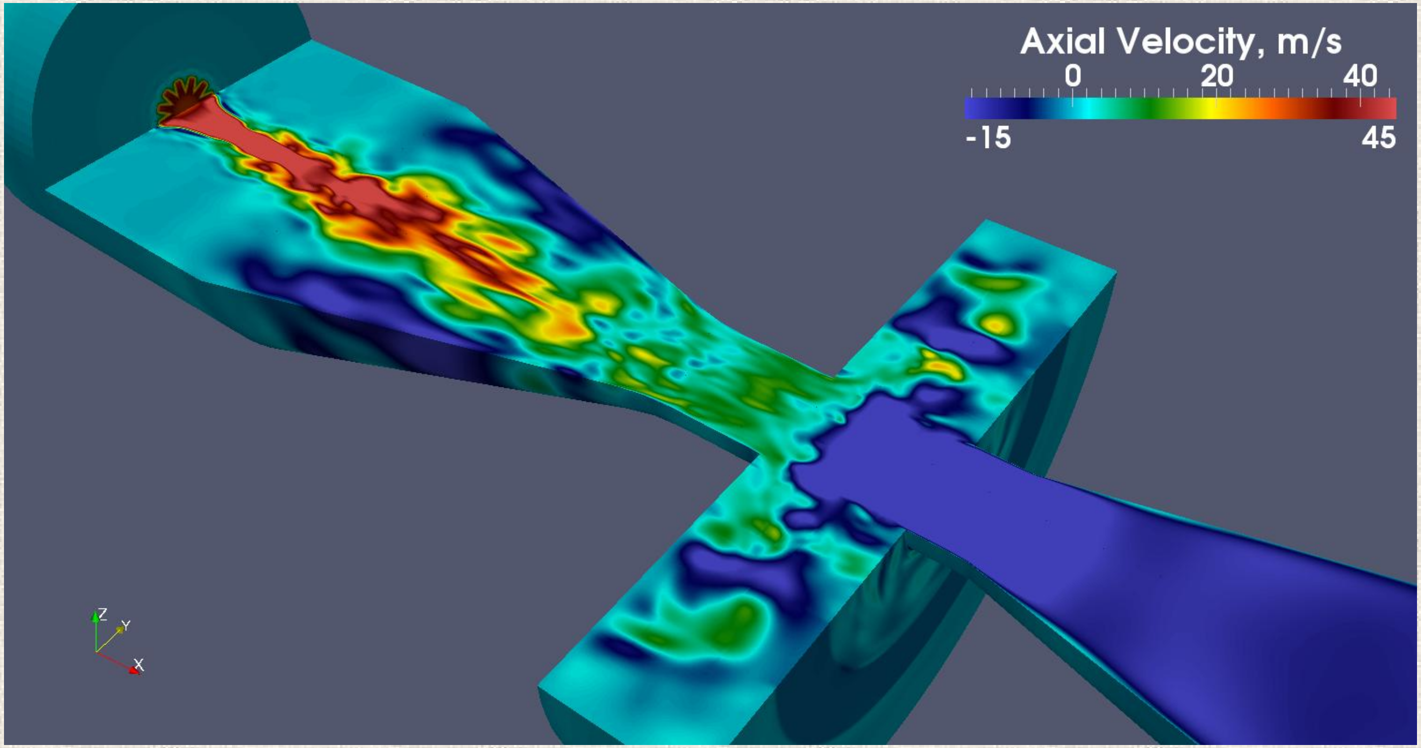
# CRAFT TECH.

## Large-Eddy Simulations of the Premixed TCF Burner

**Konstantin Kemenov, William Calhoon, Jr.**

**Combustion Research and Flow Technology, Inc. (CRAFT Tech)**
**Huntsville, AL**

# Premixed Turbulent Counterflow Burner



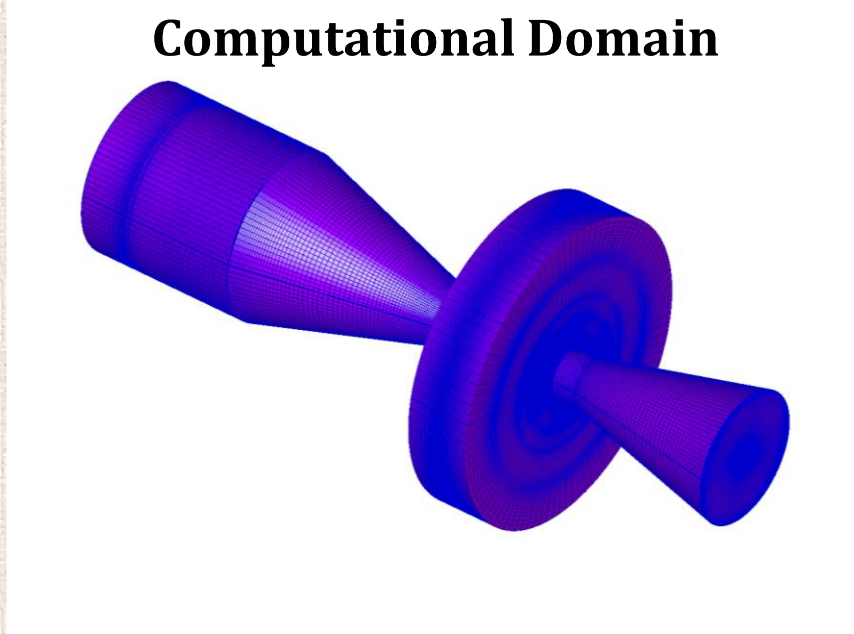

- Sandia/Yale burner studied experimentally by Coriton et al. (CF 2013)
- CRAFT Tech 1: cold $N_2$ vs. burnt at 1850K
- CRAFT Tech 2: cold $CH_4/O_2/N_2$, $\varphi = 0.85$ vs. burnt at 1850K, Turbulent Re and Ka numbers are 1050 and 5. The bulk strain rate is K=1400 1/s
- $N_2$ co-flows at both nozzles

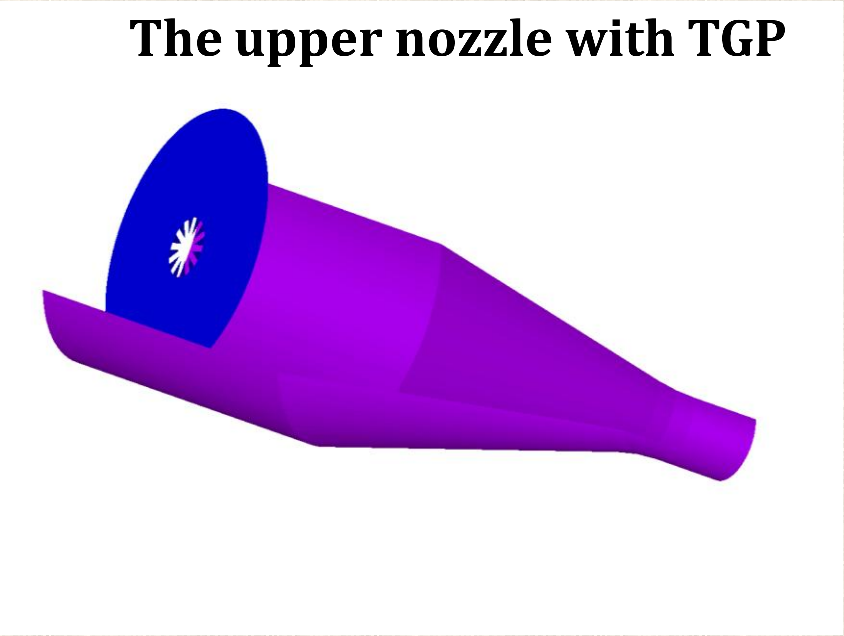
# LES Modeling

- LES of the full TCF burner configuration including: (i) the upper nozzle (with TGP), (ii) the lower nozzle, and (iii) the counterflow domain
- Vreman SGS model
- Progress variable transport equation with the source term based on the turbulent flame speed modeling
- Algebraic Pocheau model for $u_T$ (Pocheau 1994)
- LEM – CF model for the turbulent flame speed (Calhoon 2012)

$$u_T = f(\mathrm{Re}_T, \mathrm{Ka}_T, a_{LES})$$

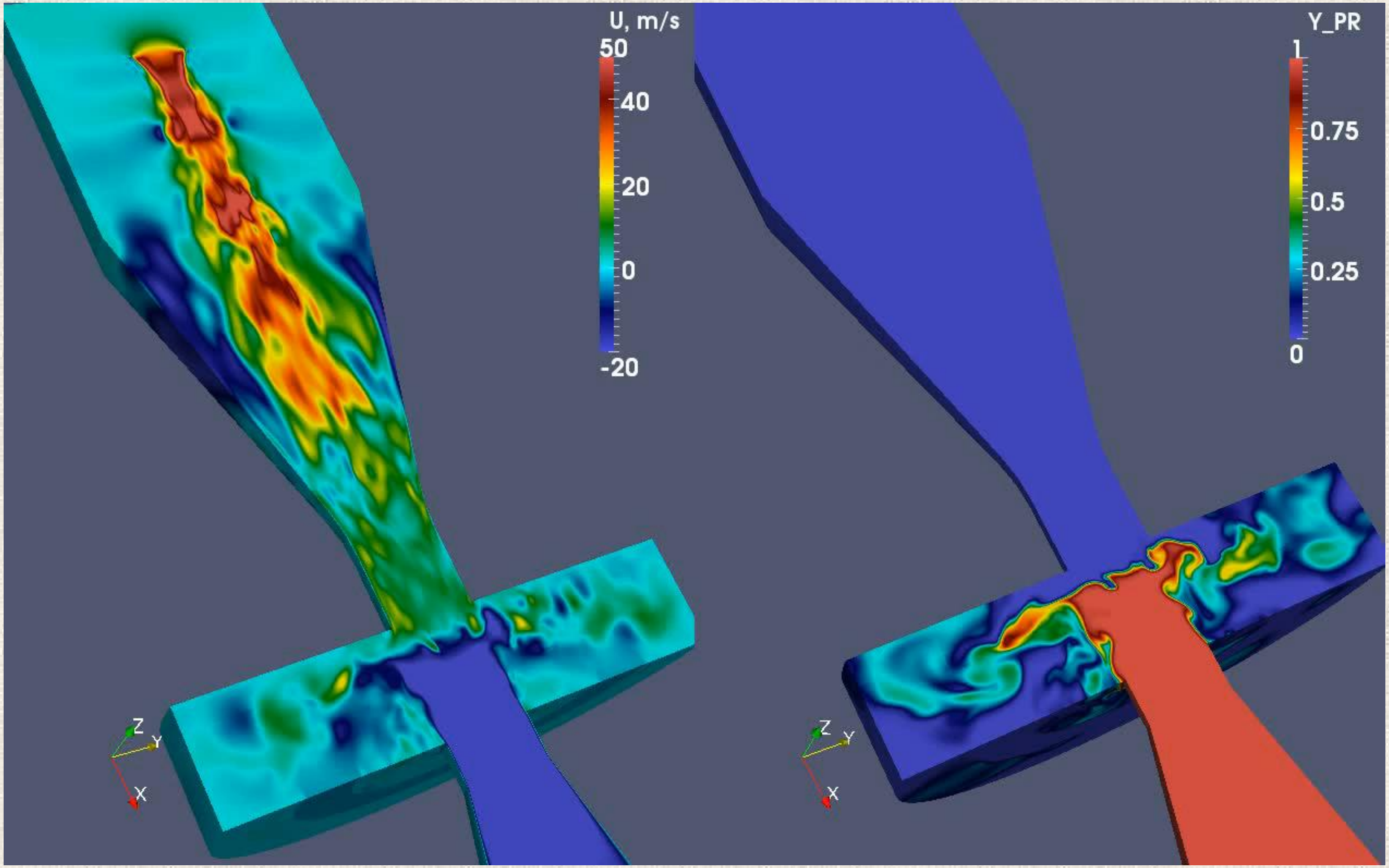
# Computational Setup



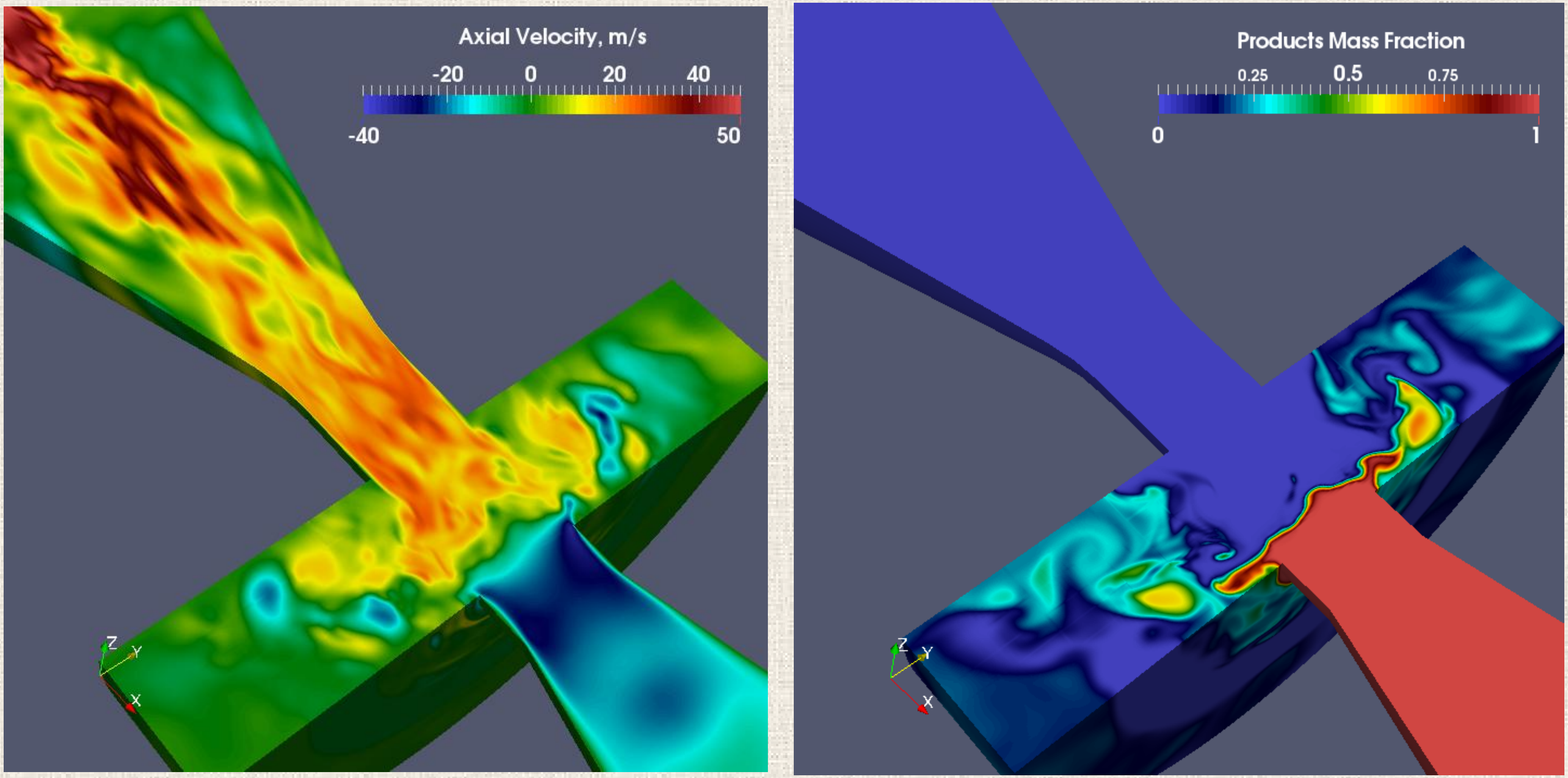




- Multi-block, high-order structural code CRAFT-CFD with preconditioning
- A central scheme with explicit filtering
- Transport equation for the subgrid TKE
- Transport equations for the reactive progress variable and $N_2$
- Two LES grids with 3.2M (G0) and 7M (G1) grid points

# CRAFT Tech. 1: $N_2$ vs. Burnt
# Animation of Velocity and Product

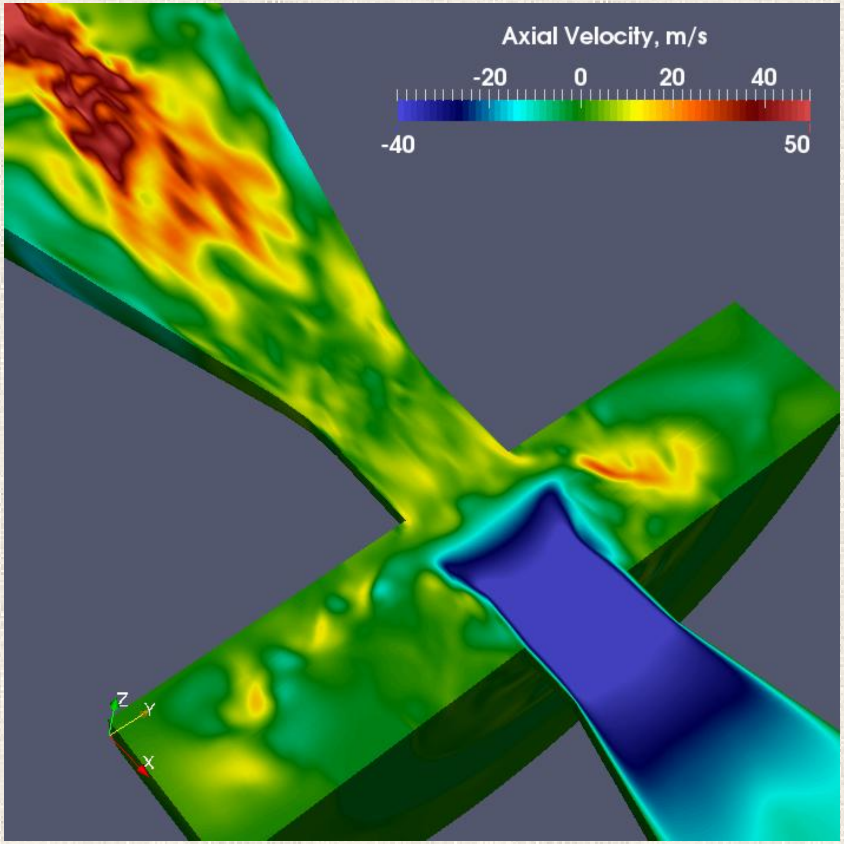


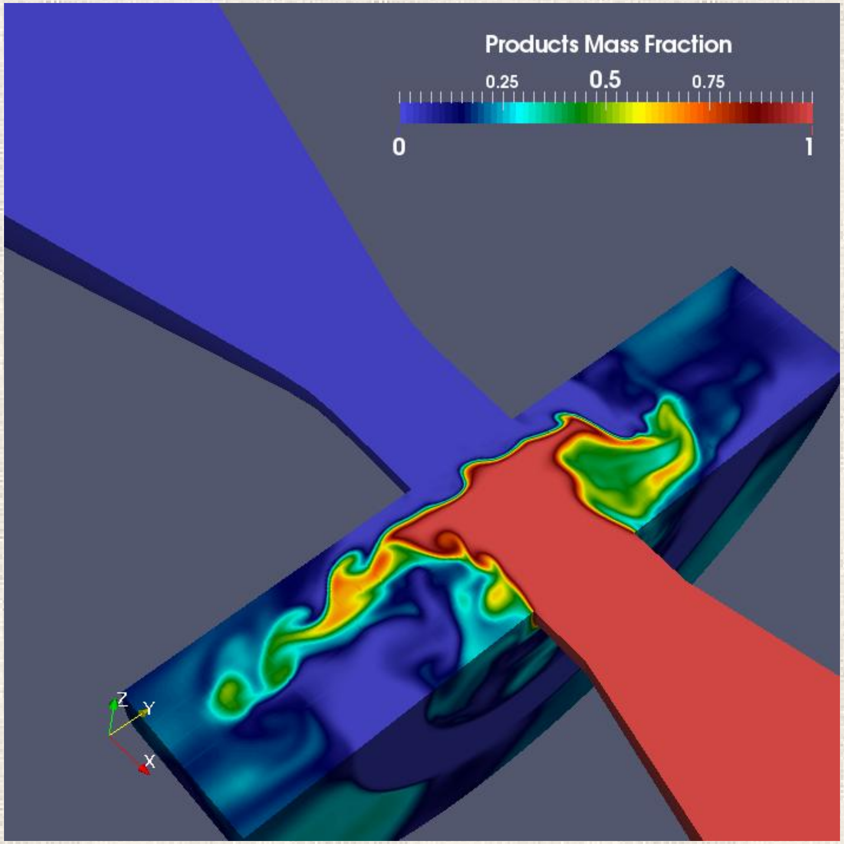
# CRAFT Tech 1: Non-reactive Case, $N_2$ vs. Burnt, G0




- ✓ **The Stagnation Interface (SI) and Gas Mixing Layer (GMLI) interface move up and <u>down</u> between the upper and lower nozzles**

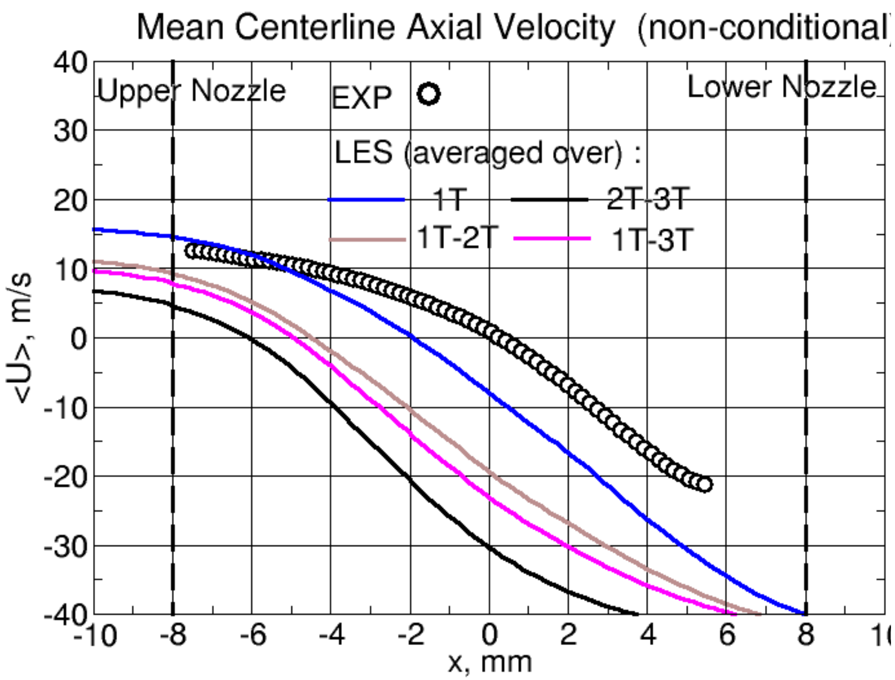
# CRAFT Tech 1: Non-reactive Case, $N_2$ vs. Burnt, G0

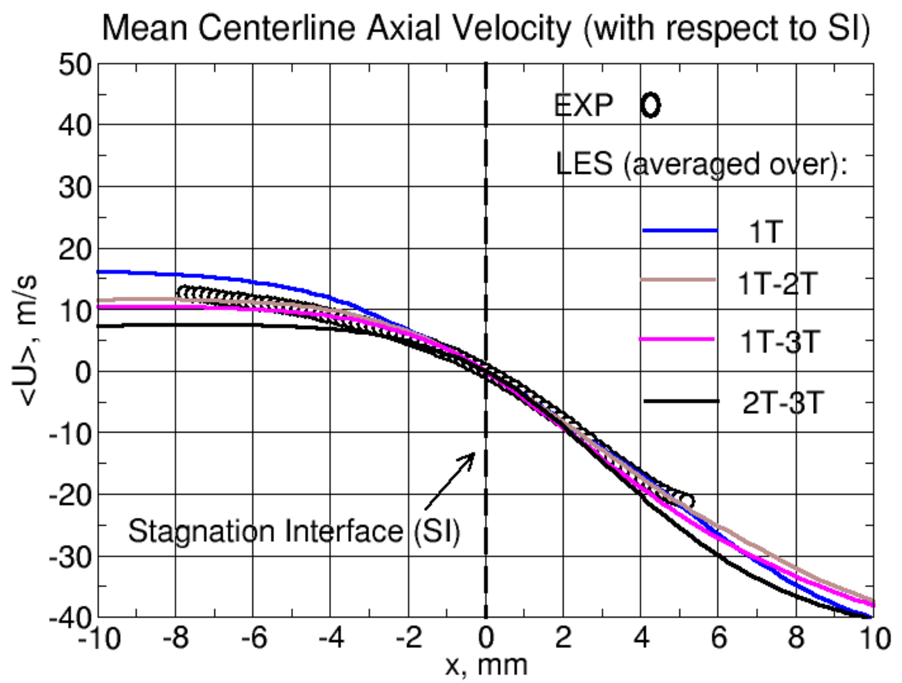



- ✓ **Stagnation Interface (SI) and Gas Mixing Layer (GMLI) interface move <u>up</u> and down between nozzles. Reduced level of the inflow turbulence at the upper nozzle is observed when the SI/GMLI is up**

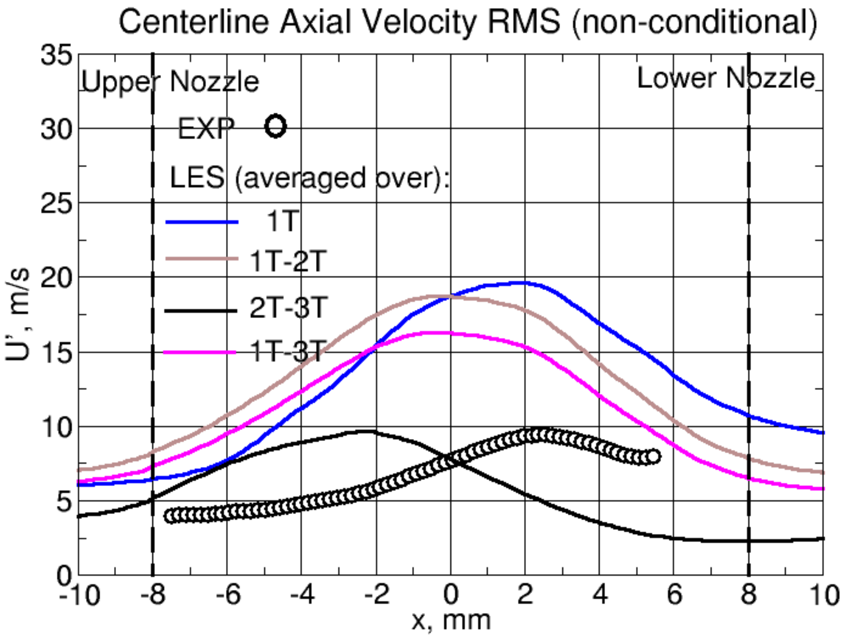
# CRAFT Tech 1: Non-reactive Case, G0
# Mean Axial Velocity

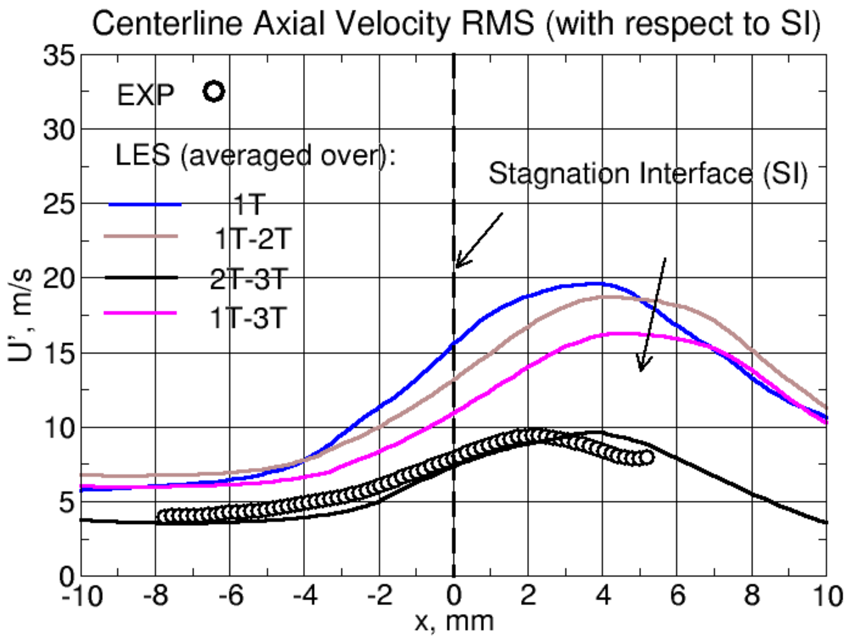



- ✓ **Unconditional mean velocity statistics strongly depend on the averaging time interval (i.e. , where the GMLI spends most of the time)**
- ✓ **Here, 1T corresponds to 45 flow through times (~ 0.5M time steps)**
- ✓ **Mean profiles are collapsed when they are plotted with respect to the SI**

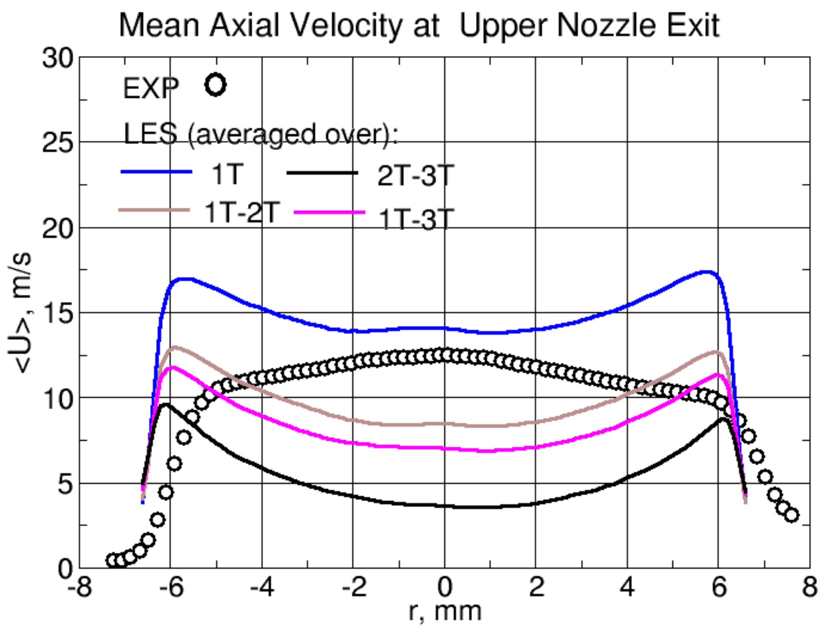
# CRAFT Tech 1: Non-reactive Case, G0
# RMS Axial Velocity

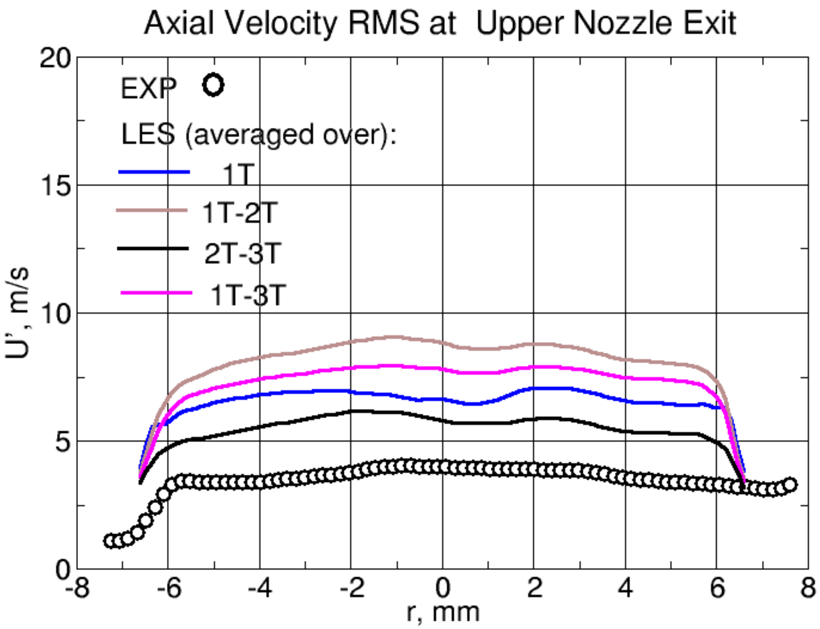



- ✓ RMS axial velocity peak values continue to drop as the averaging time interval increases and the SI moves closer to the upper nozzle
- ✓ Here, 1T corresponds to 45 flow through times (~ 0.5M time steps)
- ✓ Note that averaging over the last 90 flow through times (2T-3T) gives the best agreement with the experimental data

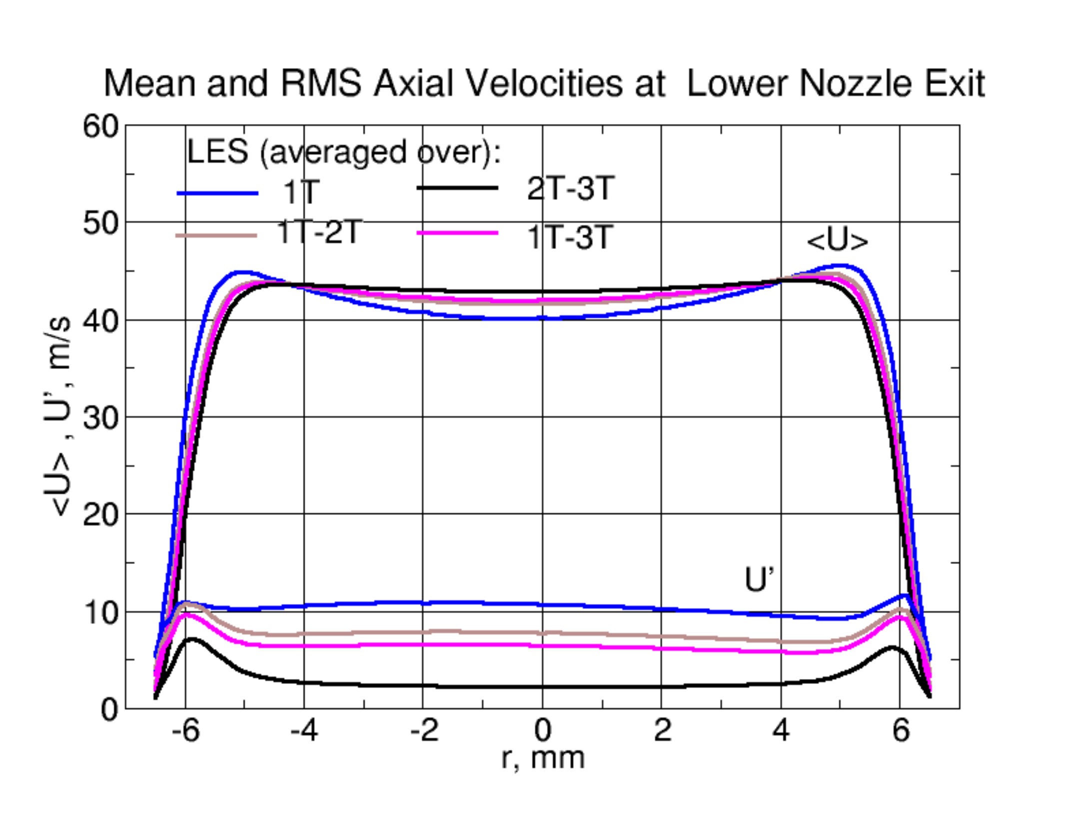
# CRAFT Tech 1: Non-reactive Case, G0
# Upper Nozzle Exit Velocity




- ✓ **Mean axial velocity is M-shaped at the upper nozzle exit and decreases in magnitude as the SI approaches the upper nozzle**
- ✓ **RMS velocity fluctuations are over-predicted as the SI spends more time closer to the upper nozzle rather than the mid-plane**

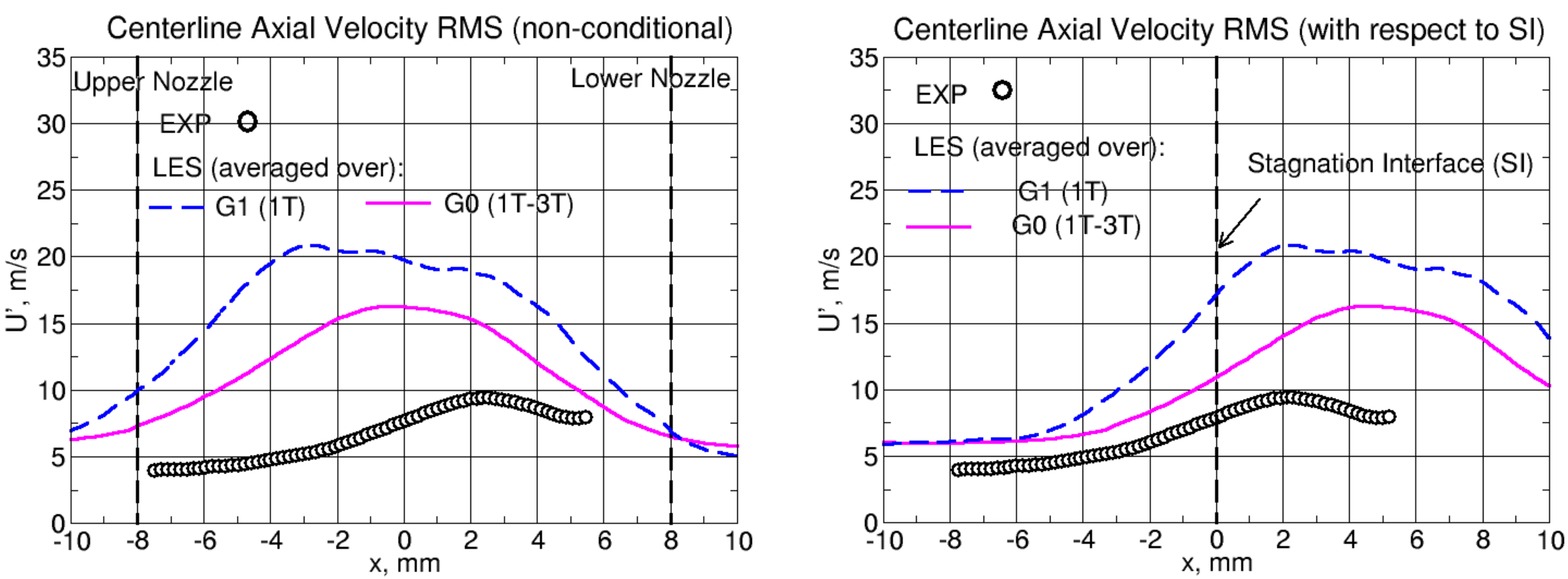
# CRAFT Tech 1: Non-reactive Case, G0
# Lower Nozzle Exit Velocity




- ✓ **Mean axial velocity (absolute value) profiles become more flat and less M-shaped as the SI moves further away from the lower nozzle**

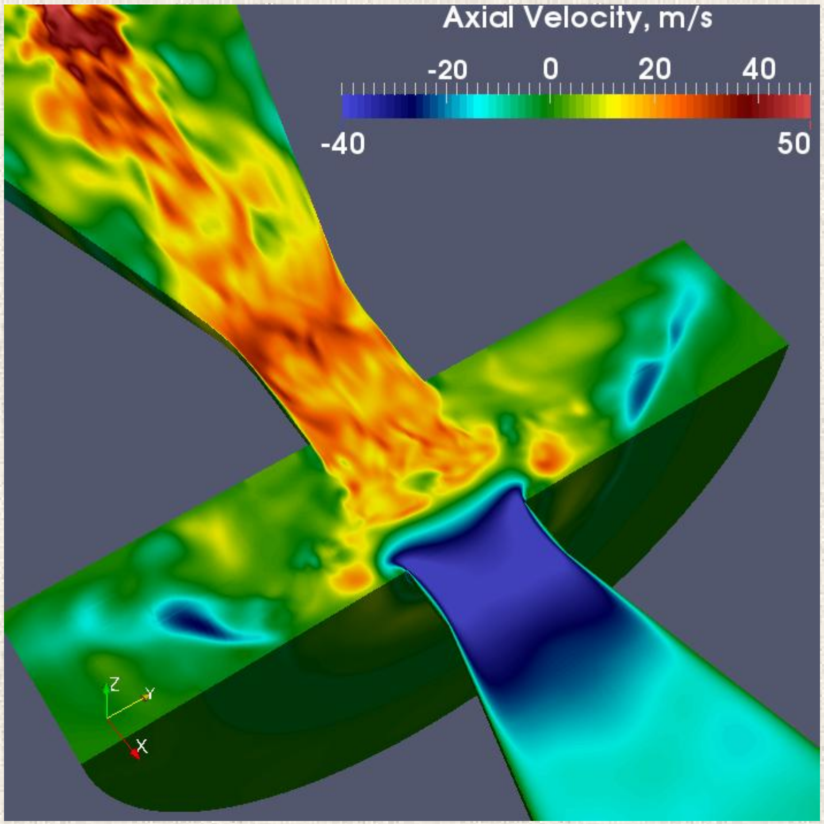
- ✓ **Relatively high level of the RMS velocity (non-turbulent) fluctuations is observed at the lower nozzle exit**

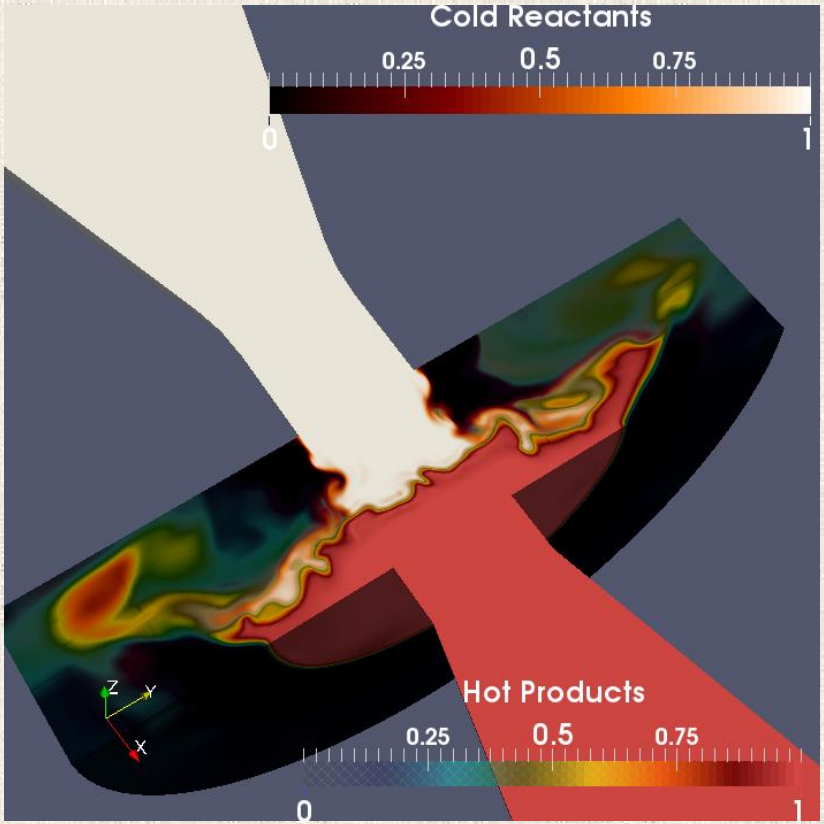
# CRAFT Tech 1: Non-reactive Case, G0 & G1
# RMS Axial Velocity




- ✓ **G1 grid case proved to be more unstable than G0 grid case**
- ✓ **The SI/GMLI topology was found to be strongly modified (or even destroyed) before experiencing an eventual recovery. This suggests the exclusion of the affected portion of LES statistics to have a meaningful comparison with the experimental data**

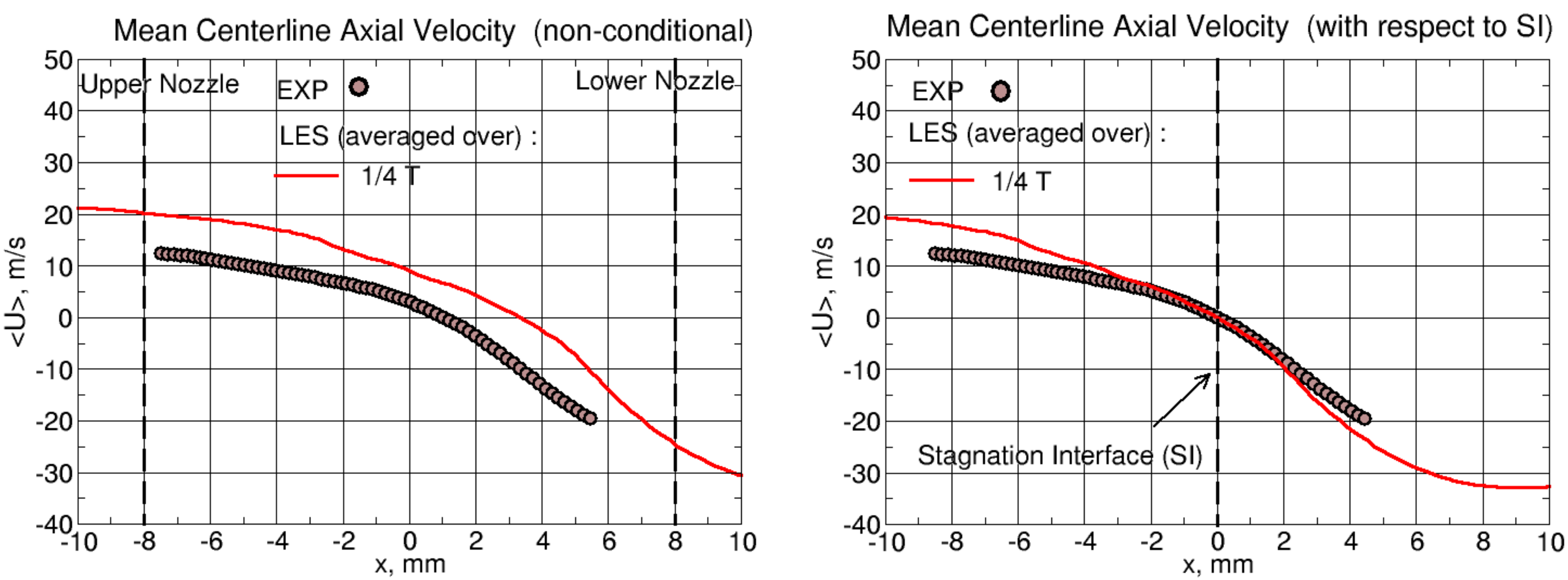
# CRAFT Tech 2: Reactive Case, G0
# Axial Velocity and Species Contours



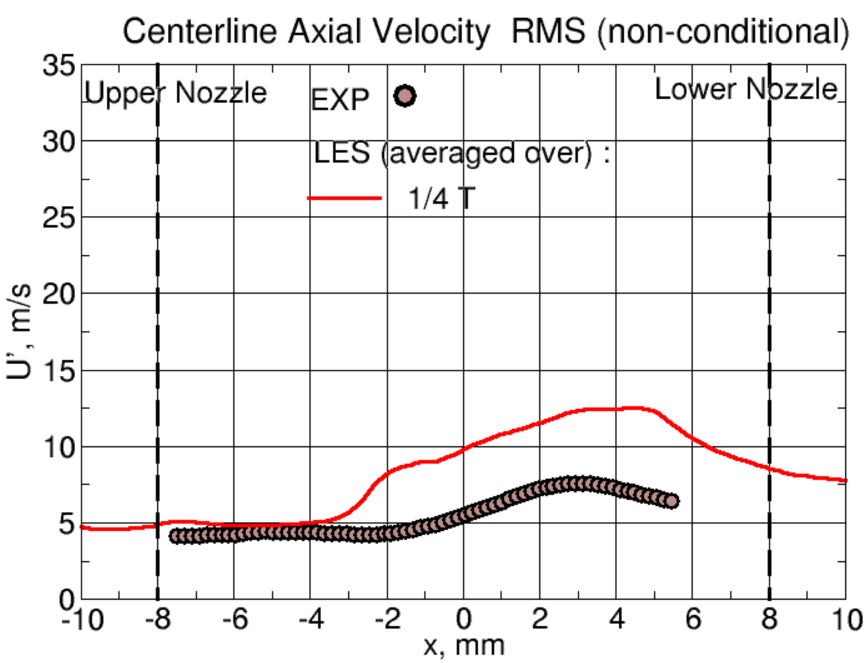

- ✓ **Typical instantaneous axial velocity and species contours after about 11 flow through times. $N_2$ contours are shown in black**
- ✓ **A simple algebraic Pocheau model is used for the turbulent flame speed**

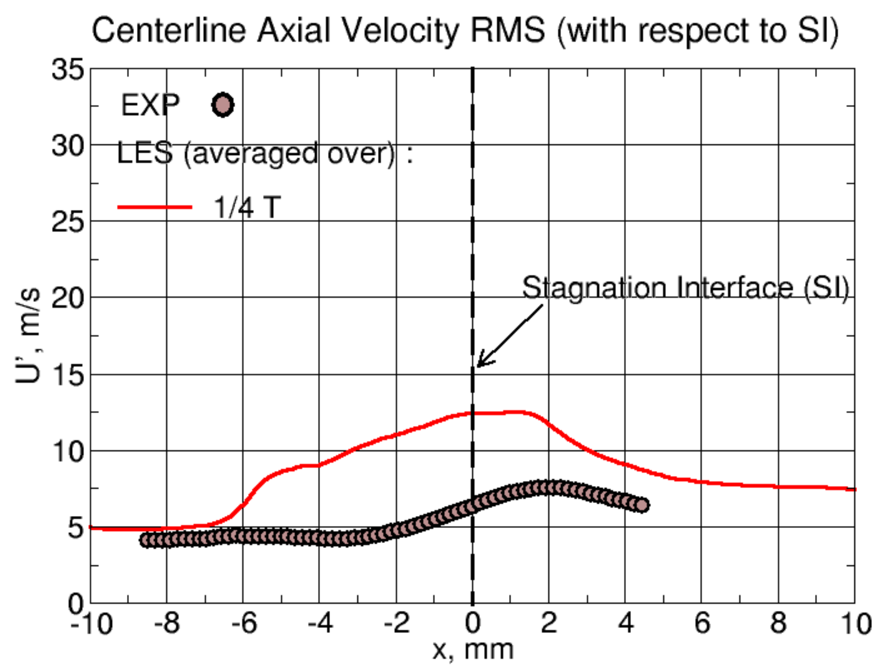
# CRAFT Tech 2: Reactive Case, G0
# Mean Axial Velocity




- ✓ **Mean centerline location of the SI is at x=3.3 mm (after about 11 flow through times)**
- ✓ **The SI has traveled down to the lower nozzle started moving back**

# CRAFT Tech 2: Reactive Case, G0
# RMS Axial Velocity




- ✓ While the RMS velocity fluctuations are still elevated they are significantly smaller than those of the non-reactive case
- ✓ Further improvement is expected as more statistics are accumulated

# CRAFT Tech.: Conclusions and Future Work

- **LES of the full premixed TCF burner geometry has been performed for the non-reactive case to study the fluid dynamical aspects of the TCF configuration. Preliminary simulation of the reactive case has also been conducted with a simple algebraic Pocheau model**

- **The results obtained demonstrate that LES is able to capture the essential features of the counter-flow dynamics for both reactive and non-reactive cases**

- **Both the GMLI and SI are found to oscillate slowly between nozzles. Unconditional statistics showed strong dependence on the averaging time interval which might suggest longer LES runs and/or alternative approaches to evaluate flow statistics (Coppola et al. 2010)**

- **Future work will focus on a study of the resolved strain rate effects on the flame front propagation with the LEM-CF model in attempt to represent extinction/re-ignition events observed in the TCF configuration experimentally**

# DUISBURG-ESSEN

## LES/FDF of IC Methane Premixed vs. Premixed

**M. Rieth[1], F. Proch[1], A. Kempf[1]**
**J.-Y. Chen[2], Peter Lindstedt[3]**

**[1]University of Duisburg-Essen**
**[2]University of California Berkeley**
**[3]Imperial College London**

# Turbulent Opposed Jet Experiments and the Simulations by the Kempf Group

## Experiments

**Imperial TOJ 1, D=25mm, $Re_{max,CH4}$=2450(?)**
**Hotwire, thermocouples, mixing, scalar dissip.**

*Mastorakos, PhD thesis, 1993*
*Sardi, Taylor, Whitelaw, J. Fluid Mech. 1998*
*Luff, Korusoy, Lindstedt, Exp. in Fluids 2003*
*Lindstedt, Luff, Whitelaw, Proc. Combust. Inst. 2007*

**Darmstadt TOJ, D=30mm, $Re_{max,CH4/air}$=7200**
**Line Raman-Rayleigh for scalar dissipation, "german engineering“, high speed PIV**

*Geyer, Kempf, Dreizler, Janicka, Proc. Combust. Inst. 2005*
*Geyer, Kempf, Dreizler, Janicka, Combust. Flame 2005*
*Böhm, Heeger, Boxx, Meier, Dreizler, Proc.Comb.Inst. 2009*
*Böhm, Stein, Kempf, Dreizler, Flow, Turb. & Combust. 2010*

**Yale TOJ, D=12.7mm, $Re_{max,CH4/air}$=8000(?)**
**Bloom mixer in a plenum**

*Coppola, Coriton, Gomez, Combust. Flame 2009*
*Coriton, Frank, Gomez, Combust. Flame 2013*

**Imperial TOJ 2, D=30mm, $Re_{(CH4/air)}$ =7500**
**Fractal plates on Darmstadt burner Premixed & against hot coflow**

*Goh, Geipel, Hampp, Lindstedt, Proc. Combust. Inst. 2013*
*Goh, Geipel, Lindstedt, Combust. Flame 2014*

## Simulations, Kempf group

**Development of combustion LES – Imperial TOJ1**
**Equilibrium chemistry**
**flowsi, 0.5 M cell, 1 CPU**

*Kempf, Forkel, Sadiki, Chen, Janicka, Proc. Combust. Inst., 2000*

**Application of combustion LES – Darmstadt TOJ**
**Flamelet chemistry, pressure coupling**
**flowsi, 3 M cell, 1 CPU**

*Geyer, Kempf, Dreizler, Janicka, Proc. Combust. Inst. 2005*
*Geyer, Kempf, Dreizler, Janicka, Combust. Flame 2005*

**Details of in-nozzle flow – Darmstadt TOJ**
**Turbulence generation, jet interaction**
**PsiPhi, 40 M cells**

*Stein, Böhm, Dreizler, Kempf, Flow, Turb. & Combust. 2011*

**Flow and combustion in new burner – Yale TOJ**
**PsiPhi, up to 70 M cells**

*Pettit, Coriton, Gomez, Kempf, Proc. Combust. Inst. 2011*

**Development of hybrid Flamelet/FDF method in Darmstadt TOJ**
**Combustion, non-flamelet chemistry, extinction**
**PsiPhi, 1.7 M cells, 5 M particles, 4-step chemistry**

*Rieth, Chen, Proch, Kempf, 2013/2014, to be submitted*

**Premixed flame in Imperial TOJ2**
**Fractal plate generated turbulence, premixed (& products)**
**PsiPhi, 1.7 M cells, 8 M particles**

*Rieth, Chen, Proch, Lindstedt, Kempf, work in progress*

# Duisburg-Essen 1:
# Darmstadt Rich Methane/air vs. Air

- **Darmstadt TOJ** (Geyer et al. 2005, Böhm et al. 2010)
  - Partially premixed turbulent opposed jet flame
  - Nozzle 1: methane ($\phi$=2.0, 3.18), nozzle 2: air
  - Perforated plate generated turbulence ($Re_t$=~90, $U_b$=3.4 m/s)
  - Measurements used for comparison:
    - ✓ Velocity statistics (PIV)
    - ✓ Temperature (Raman/Rayleigh)
  - Simulation contains flow between perforated plates
  - Methane with $\phi$=2.0 simulated

# Duisburg-Essen 2: Imperial Premixed/Premixed

- **Imperial TOJ (Goh, Geipel, Lindstedt 2014)**
  - Lean premixed turbulent opposed jet flame
  - Nozzle 1&2: methane, ethylene, propane ($\phi$=0.7, 0.8, 0.9)
  - Fractal grid generated turbulence ($Re_t$=130-318, $U_b$=4.8 m/s)
  - Measurements used for comparison:
    - ✓ Velocity statistics (PIV)
    - ✓ Progress variable (PIV with density segregation method)
  - Simulation contains flow between fractal grids
  - Methane with $\phi$=0.9 simulated

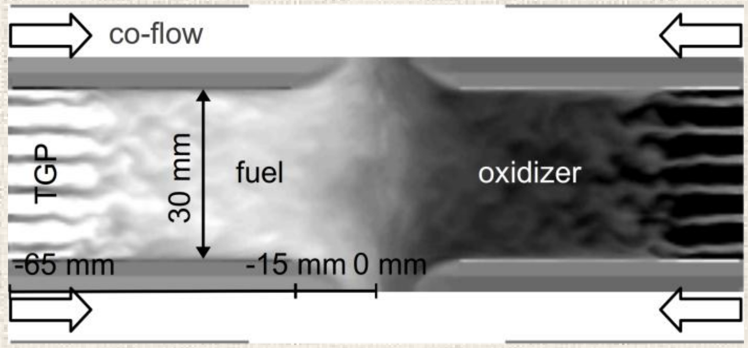
# Details of the LES/FDF Models

- LES/FDF technique
  - LES
    - ✓ Low Mach number, variable density
    - ✓ Sigma model for subgrid-scale closure ($C_m$=3.0)
  - FDF (Raman, Pitsch 2007)
    - ✓ 4-step chemistry (Peters, Kee 1987)
    - ✓ Parab. edge reconstruction method PERM (McDermott, Pope 2008)
    - ✓ Modified Curl mixing model ($C_m$=2.0) (Janicka et al. 1979)
    - ✓ Consistency by density coupling

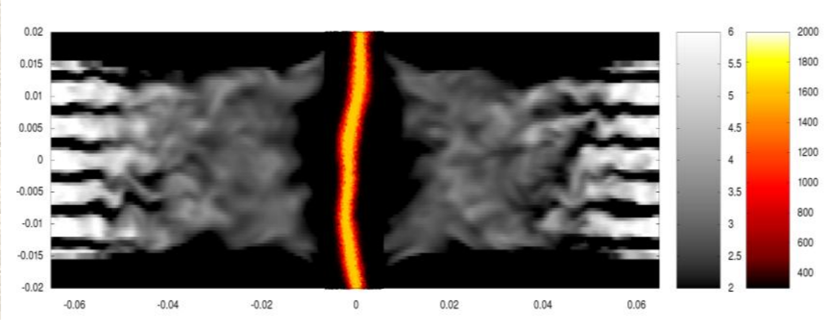
# Details of the Numerical Methods

- **LES/FDF technique**
  - **LES**
    - ✓ 3rd order Runge-Kutta (RK) time integration
    - ✓ 2nd order spatial discretization (CDS/TVD)
    - ✓ Predictor-Corrector scheme
    - ✓ Equally sized cubic cells
  - **FDF**
    - ✓ 1st order Euler-Maruyamma embedded in LES RK scheme
    - ✓ 2nd order tri-linear interpolation scheme, PERM
    - ✓ Filtering of particle fields for density coupling
    - ✓ Movement, mixing and reaction in each RK sub-step
    - ✓ Particles only used in flame zone

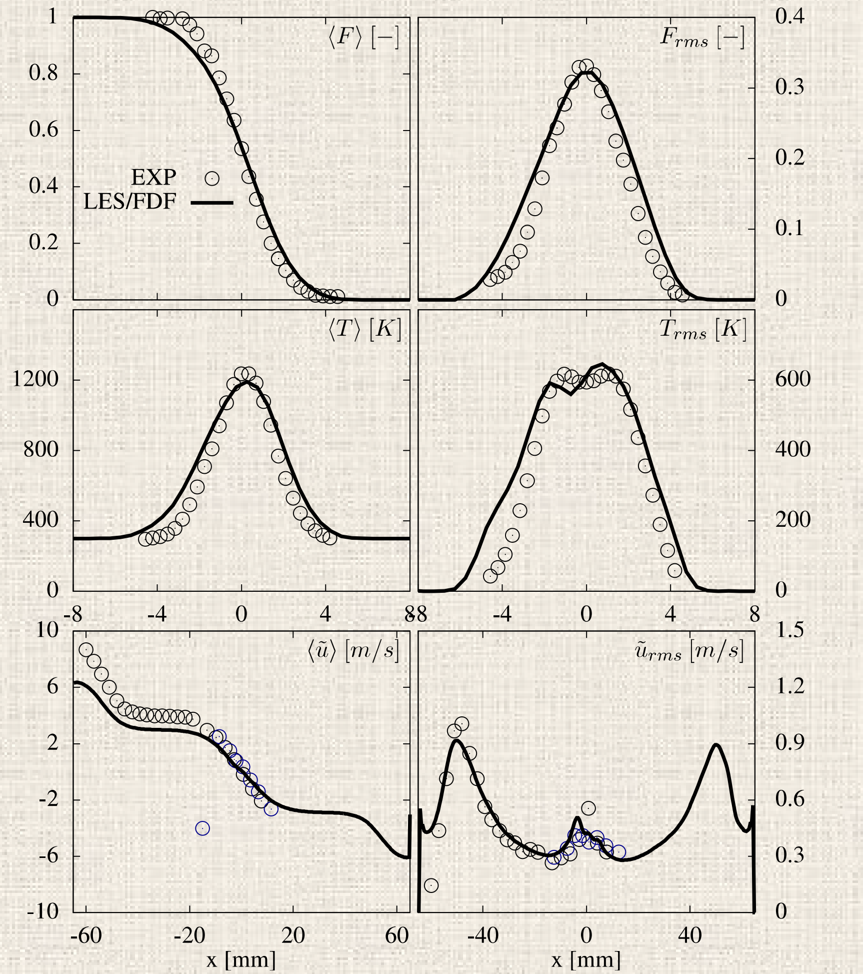
# Duisburg-Essen 1: Darmstadt TOJ LES/FDF




- **Domain size: 130x40x40mm$^3$**
- **1.7x10$^6$ cells of 0.5mm$^3$, 6x10$^6$ particles (~25 per cell)**
- **Hybrid chemistry: combined flamelet/finite rate chemistry FDF**



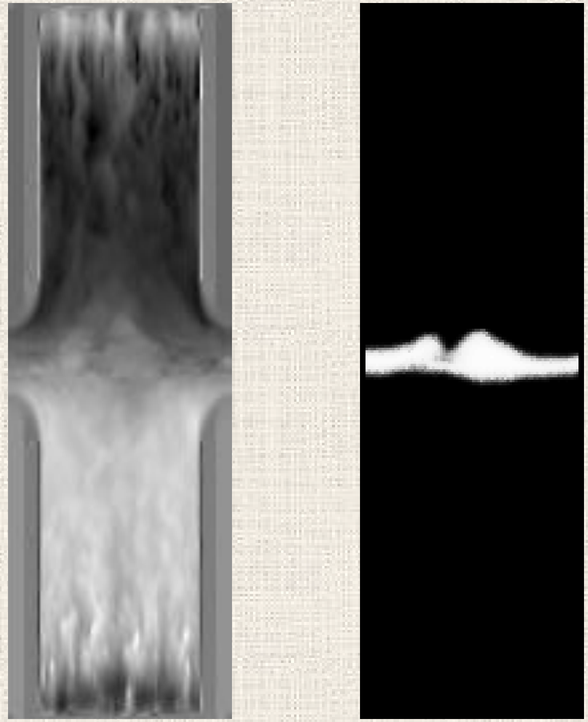
**Axial velocity (U), particle temperature (T)**



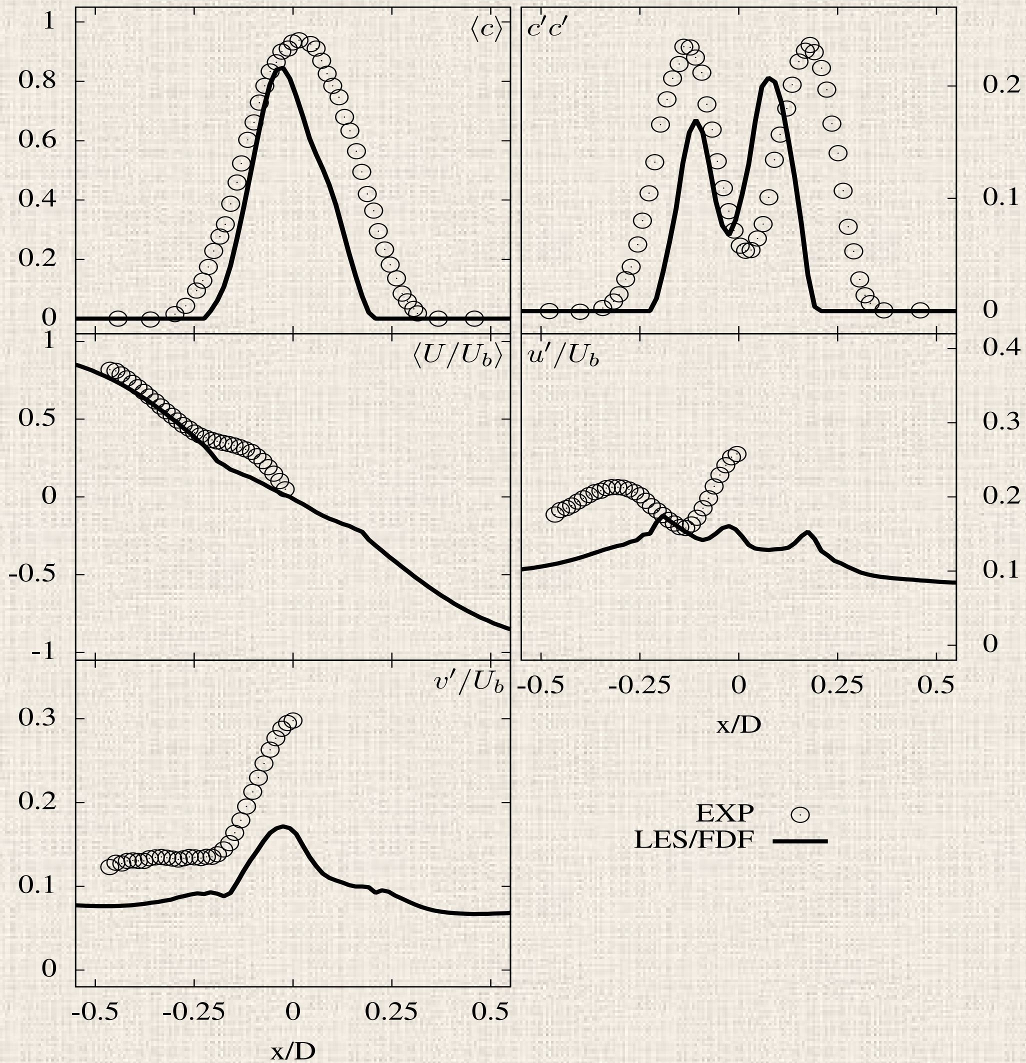

**Mean and rms of mixture fraction (top row), temperature (middle row) and axial velocity (bottom row)**

# Duisburg-Essen 2: Imperial TOJ LES/FDF

**PRELIMINARY**



Axial velocity (U), progress variable (C)



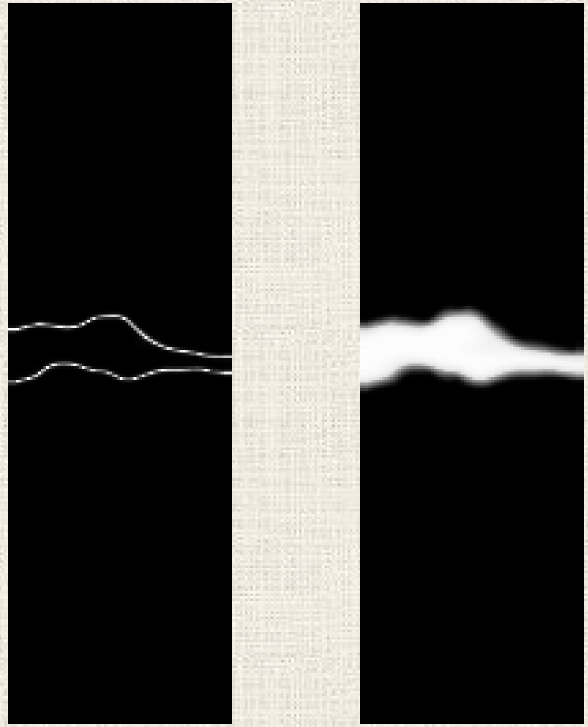

- Domain size: 130x40x40mm$^3$
- 1.7x10$^6$ cells of 0.5mm$^3$, 6x10$^6$ particles (~25 per cell)

Top row: mean and variance of progress variable

Middle row: mean and rms of axial velocity

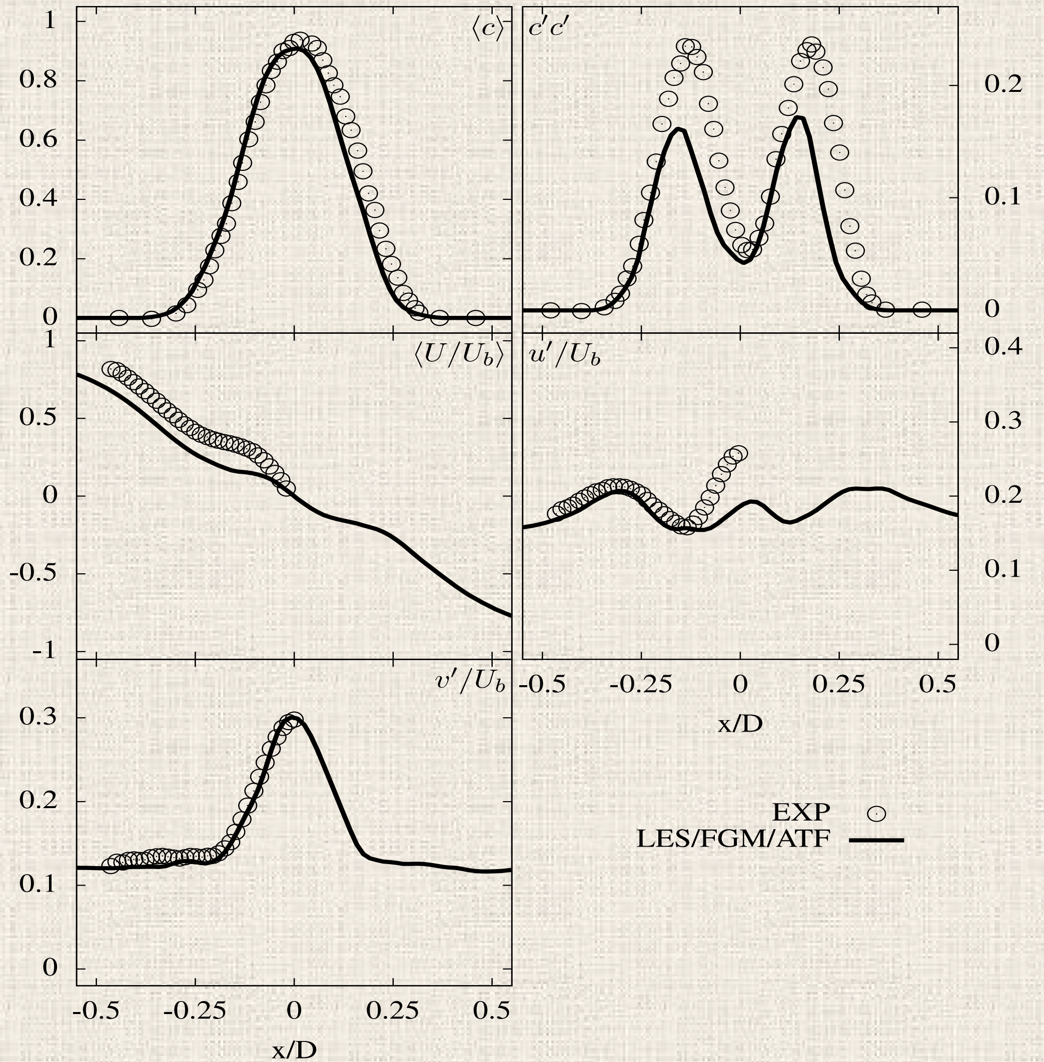
Bottom row: rms of radial velocity

# Duisburg-Essen 2: Imperial TOJ LES/FGM/ATF



**Progress specific reaction rate ($r_p$), progress variable (C)**

- **Domain size: 130x40x40mm$^3$**
- **1.7x10$^6$ cells of 0.5mm$^3$, no particles**

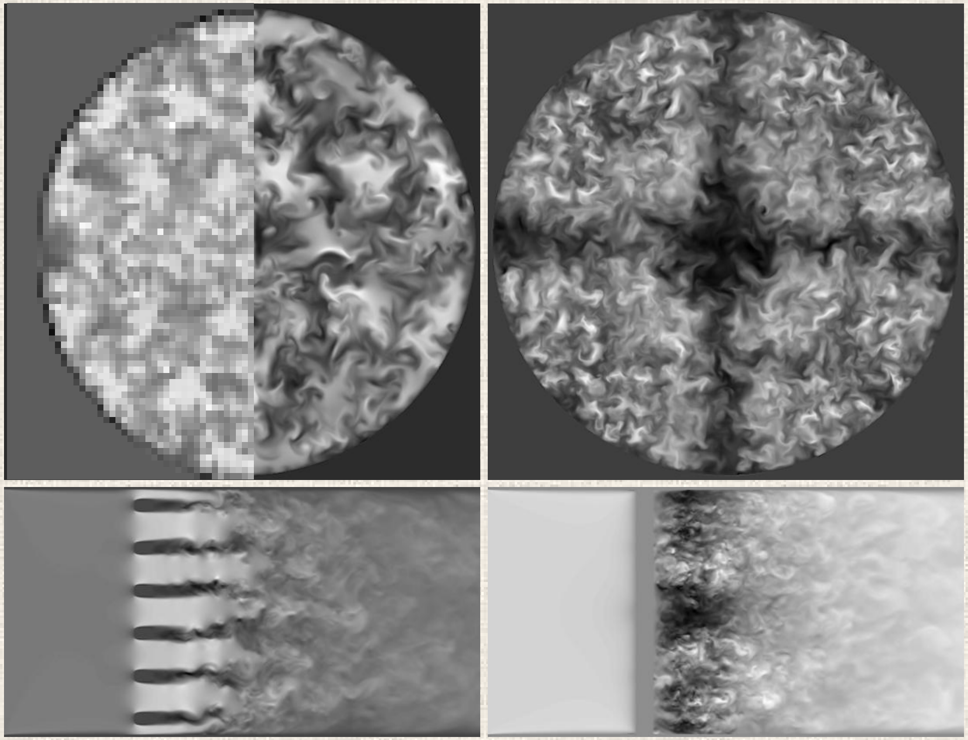



**Top row: mean and variance of progress variable**

**Middle row: mean and rms of axial velocity**

**Bottom row: rms of radial velocity**

# LES/DNS (single nozzle)



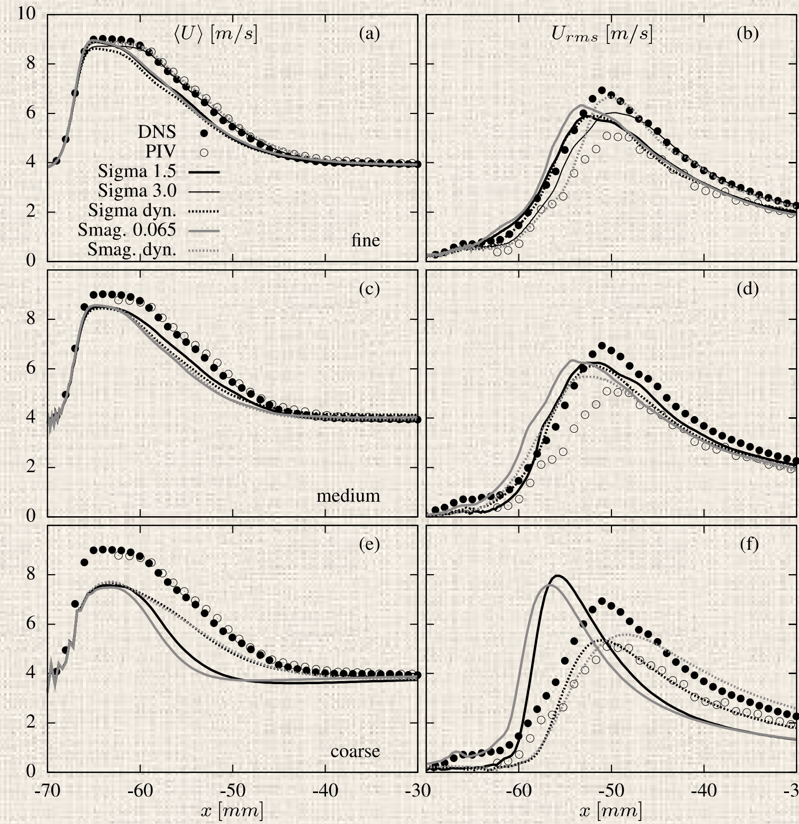
**Left: perforated plate (0.4 mm/0.05 mm grid)**

**Right: fractal grid (0.05 mm grid)**

**Left: $U_b$=3.4 m/s, right: $U_b$=4.0 m/s**

**Top: Axial velocity 10 mm downstream of grid**

**Bottom: Axial vel. in plane containing the centerline**




**Perforated plate mean and rms of axial centerline velocity for 0.1 mm, 0.2 mm and 0.4 mm grids (Rieth et al. 2014)**

# Duisburg-Essen:
# Conclusions and future work

- **Agreement between LES/FDF and experiment:**
  - **D-E 1: Darmstadt TOJ: good, but extinction limit too low**
  - **D-E 2: Imperial TOJ: results need to be improved**

- **Extend simulations to:**
  - **Other available equivalence ratios**
  - **Different fuels (ethylene, propane)**

# CORNELL

## Numerical Simulations of Highly-Turbulent Counterflow Flames (TCFs) in Non-Premixed & Premixed Modes

**Contributors:**

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# Overview

## ❑ Simulation approach

- LES-PDF methodology

## ❑ Simulations of Yale burner

- Cornell 1: Isothermal flow – $N_2$ vs. $N_2$
- Cornell 2: Non-premixed flame – $CH_4/N_2$ vs. $O_2$
- Cornell 3: Inert/Burnt – $N_2$ vs. Hot product stream
- Cornell 4: Premixed/Burnt – $CH_4/O_2/N_2$ vs. Hot product stream

## ❑ Comparisons made

- Velocity statistics (1,2,3,4)
- Mean OH mass fraction (non-premixed case, 2)
- Conditional /unconditional mean progress variable (premixed case, 4)

# Numerical Implementation

## ❑ LES: NGA code

- Transport equations for mass and momentum based on the filtered velocity field are solved on a structured cylindrical grid
- Pressure Poisson equation is solved to enforce continuity
- Two-way coupling between NGA and HPDF codes
  - ✓ Transport equation for specific volume is solved in NGA
  - ✓ Source term computed from the HPDF particle data

## ❑ PDF modeling: HPDF code

- Turbulence-chemistry interactions modeled using composition PDF method
- Monte Carlo particle/mesh method
- Composition variable ($\Phi$) consists of $n_s$ species mass fractions and enthalpy
- Each particle's position and composition is evolved by a set of Stochastic Differential Equations (SDEs) involving transport, mixing and reaction steps

# Models Used

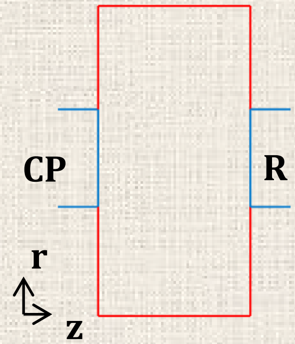
- **LES: Lagrangian dynamic sub-grid scale model is used to obtain the turbulent viscosity and turbulent diffusivity**

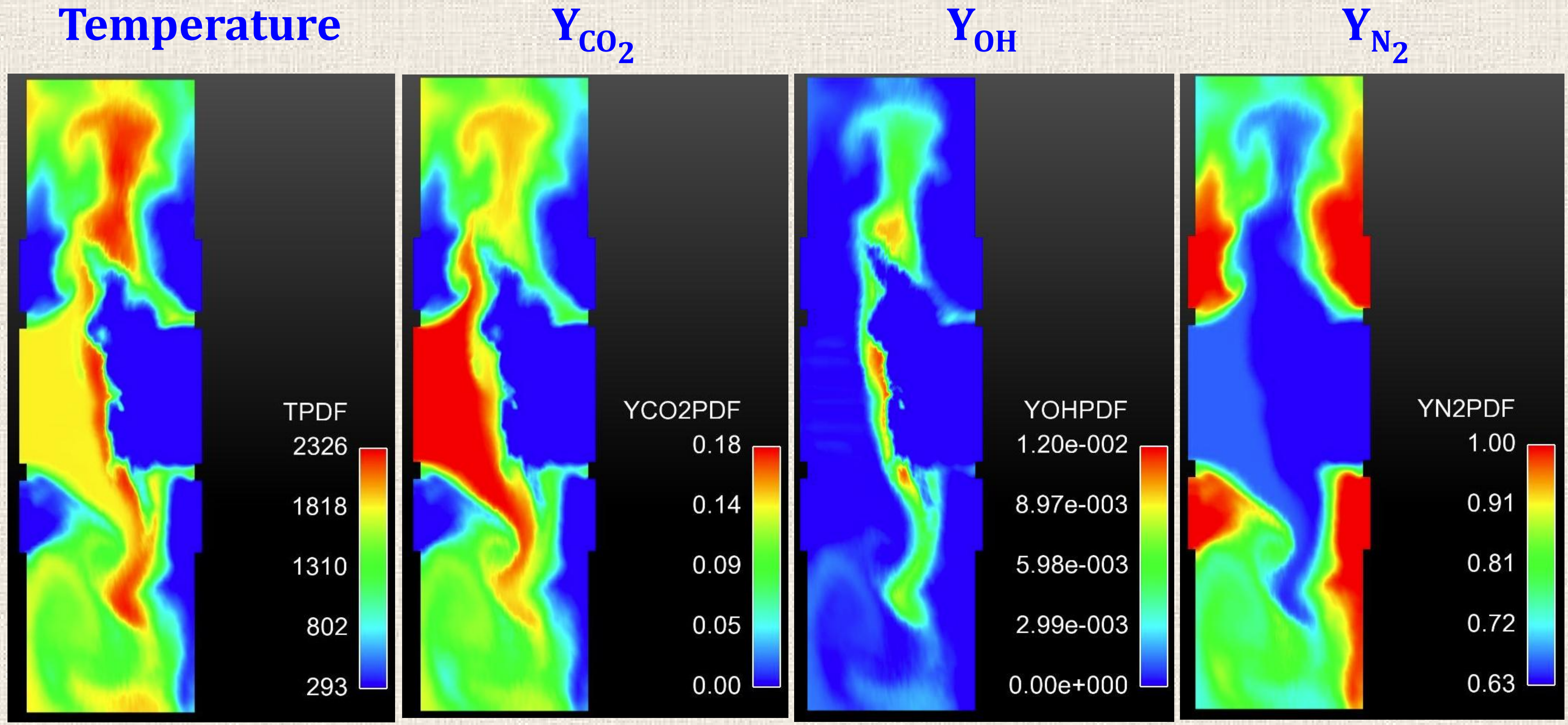
- **PDF:**
  - Turbulent transport modeled using gradient-diffusion hypothesis involving turbulent diffusivity
  - IEM mixing model

- **Molecular transport:**
  - Unity Lewis number
  - Thermal diffusivity obtained from CHEMKIN's TRANLIB

- **Chemistry: 16-species ARM1 mechanism for methane**

# Cornell 4: Premixed vs. Burnt Instantaneous Contour Plots



# Inflow Velocity BCs

## Top Nozzle Exit

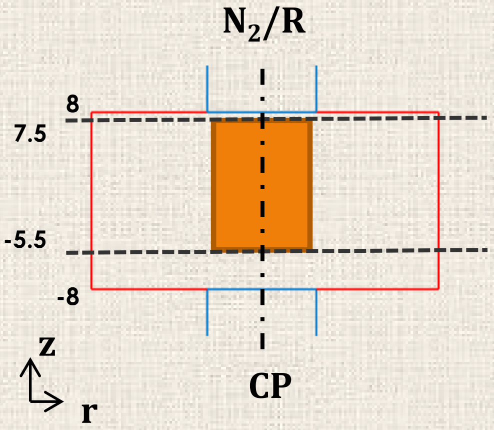
- Velocity time series data provided by Dr. Pettit using “PsiPhi” LES code (Imperial College) are scaled to match experimental $Re_t$

$$U_{i,React}(r,\theta,t)=\langle U_i(r)\rangle_{exp,React}+\alpha_i(r)\left[U_{i,nozzle}(r,\theta,\beta t)-\langle U_i(r)\rangle_{nozzle}\right]$$

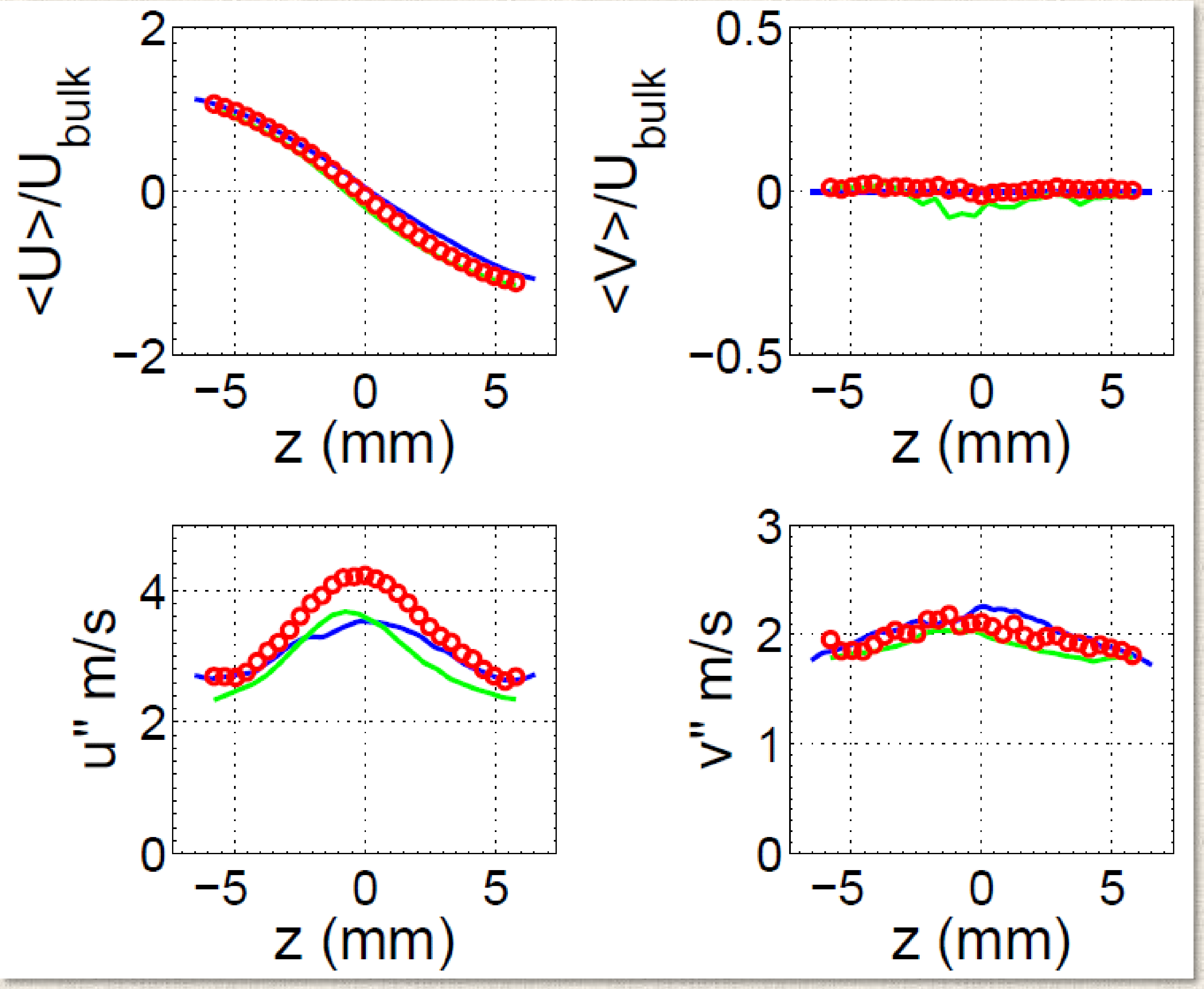
- **Notation:**
  - $\alpha_i(r)$: to match the r.m.s velocity; $\beta = T_{nozzle}/T_{React}$: to match the turbulent length scale/time scale;
  - $U_{i,nozzle}$ is Pettit’s nozzle simulation velocity time-series data;
  - $\langle U_i(r)\rangle_{exp,React}$ is the velocity mean from experiments available at 0.5 mm downstream of the nozzle exit;
  - $U_{i,React}$ is the resultant modified velocity time-series data

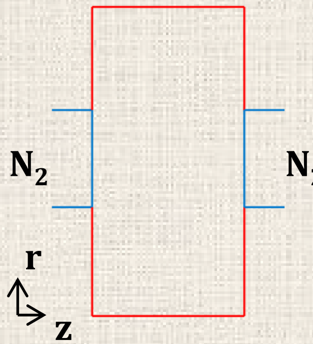
## Bottom Nozzle Exit

- Hot product stream is assumed to be laminar (no TGP)
- Experimental data available at 2.5 mm above the product inlet side are scaled
- Axial velocity profile (<U>) is scaled to achieve the required volume flow rate
- Radial velocity profile (<V>) is scaled such that the mean stagnation plane is established at the mid-plane

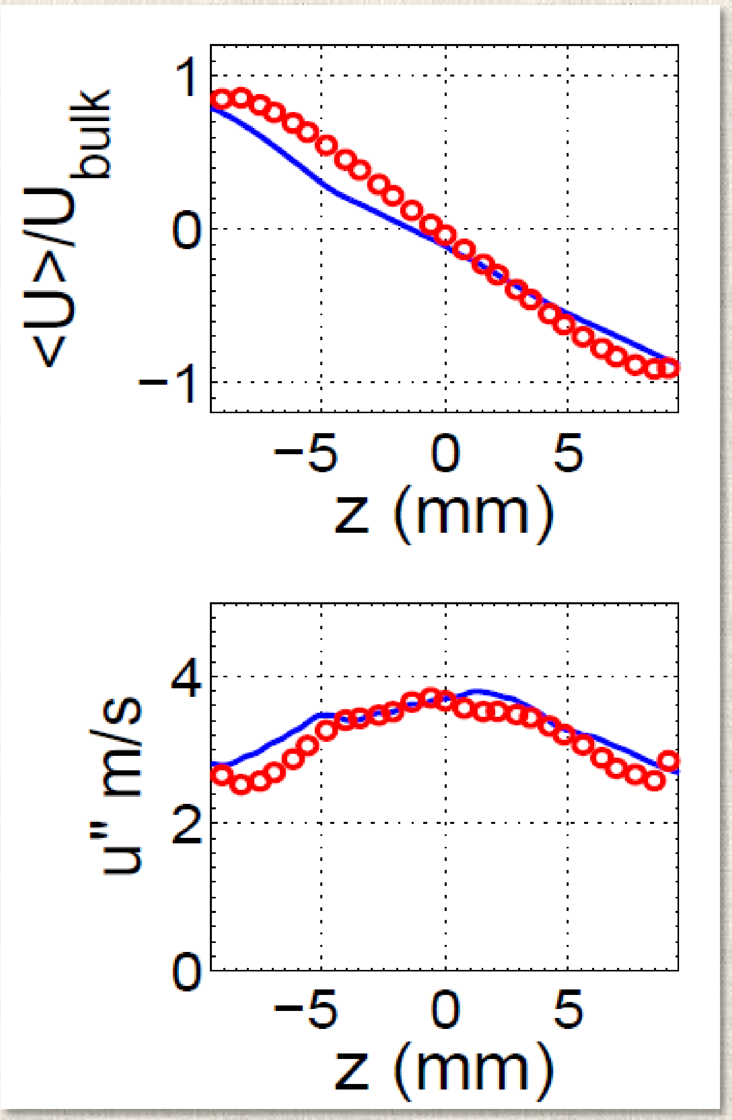


# Cornell 1: Cold $N_2$ vs. $N_2$
# Centerline Mean and RMS Velocity



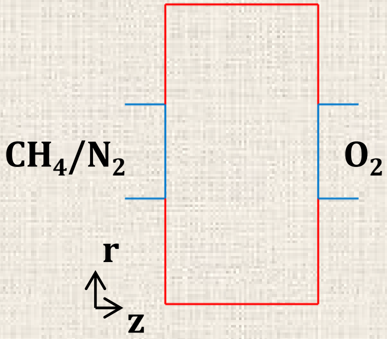



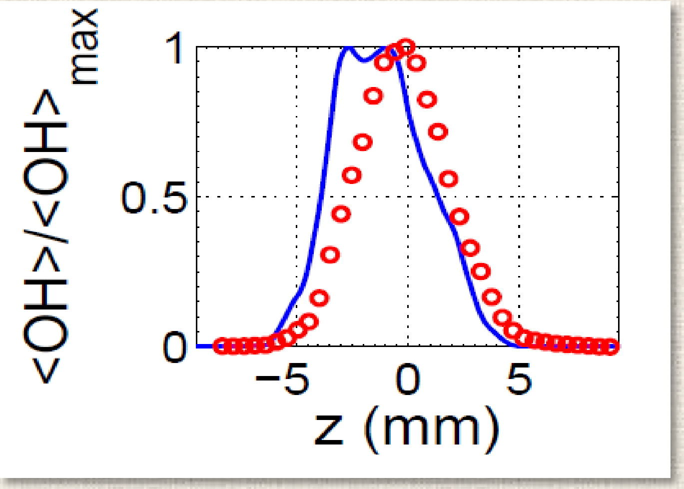

# Cornell 2: Non-Premixed Centerline Velocity and OH



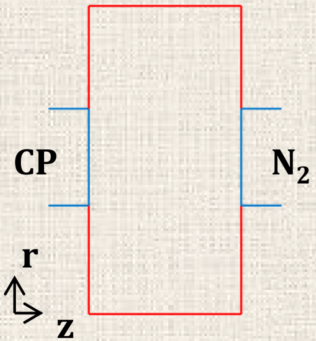

– Simulations

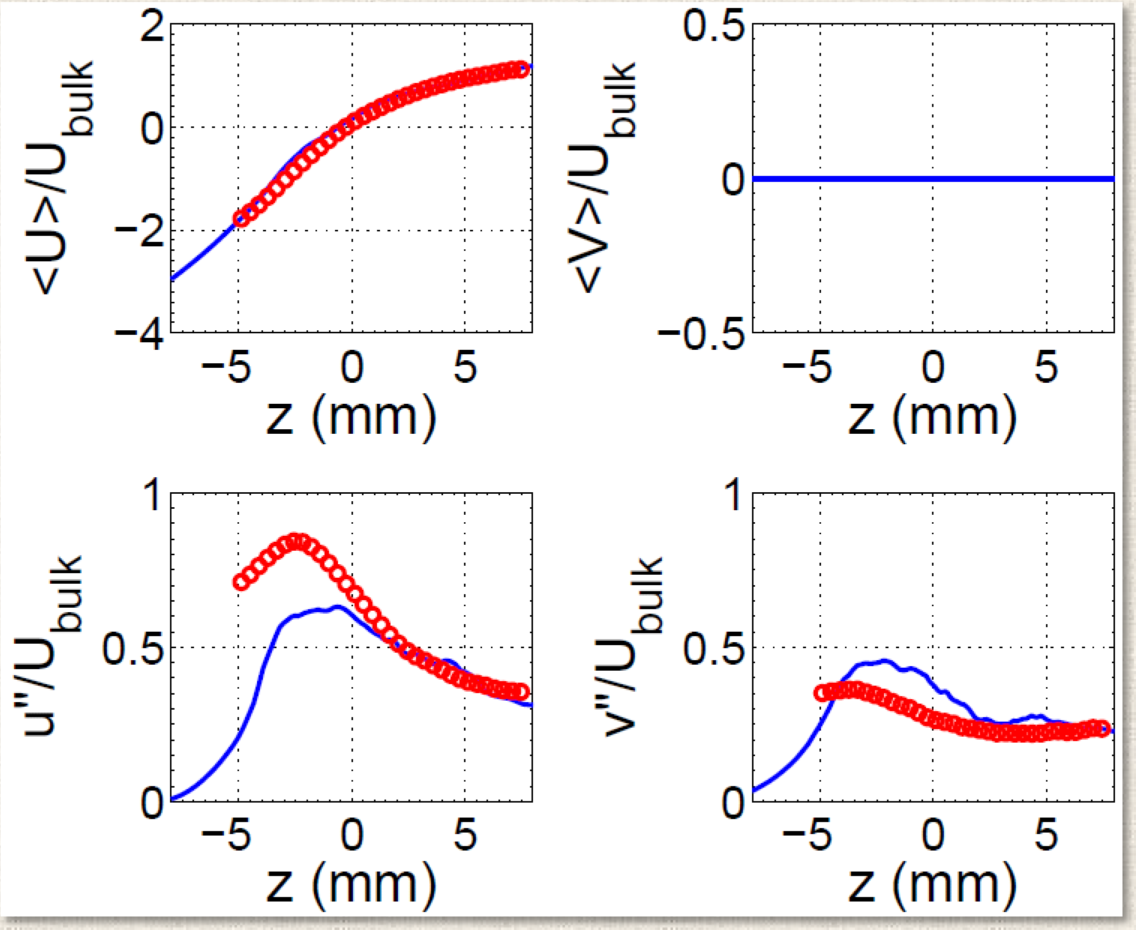
o Experiments



# Cornell 3: $N_2$ vs. Burnt
# Centerline Velocity Mean and RMS

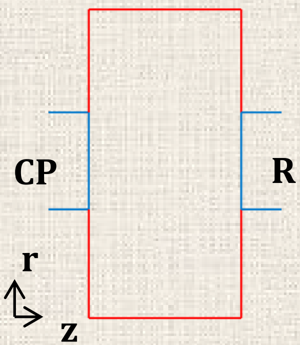


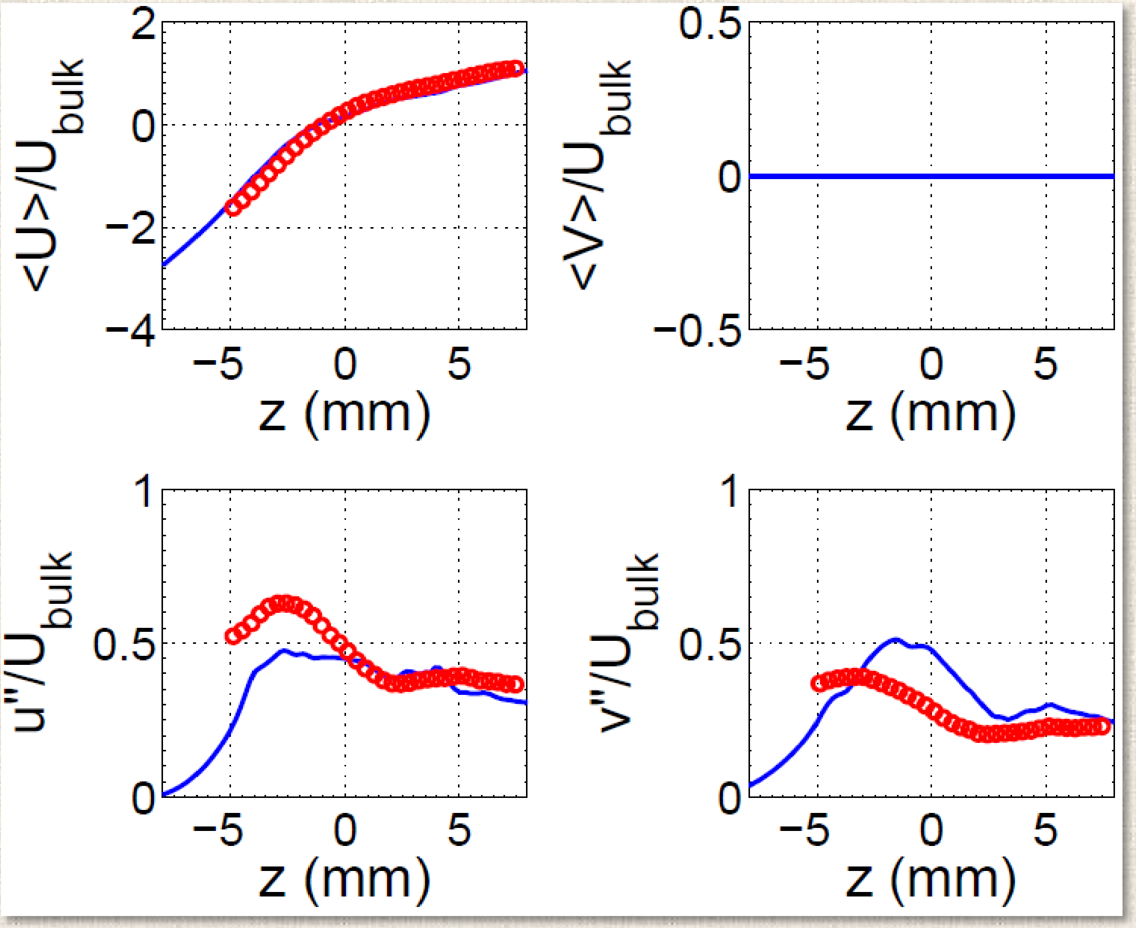




**– Simulations**

**o Experiments**

# Cornell 4: Premixed vs. Burnt
# Centerline Velocity Mean and RMS

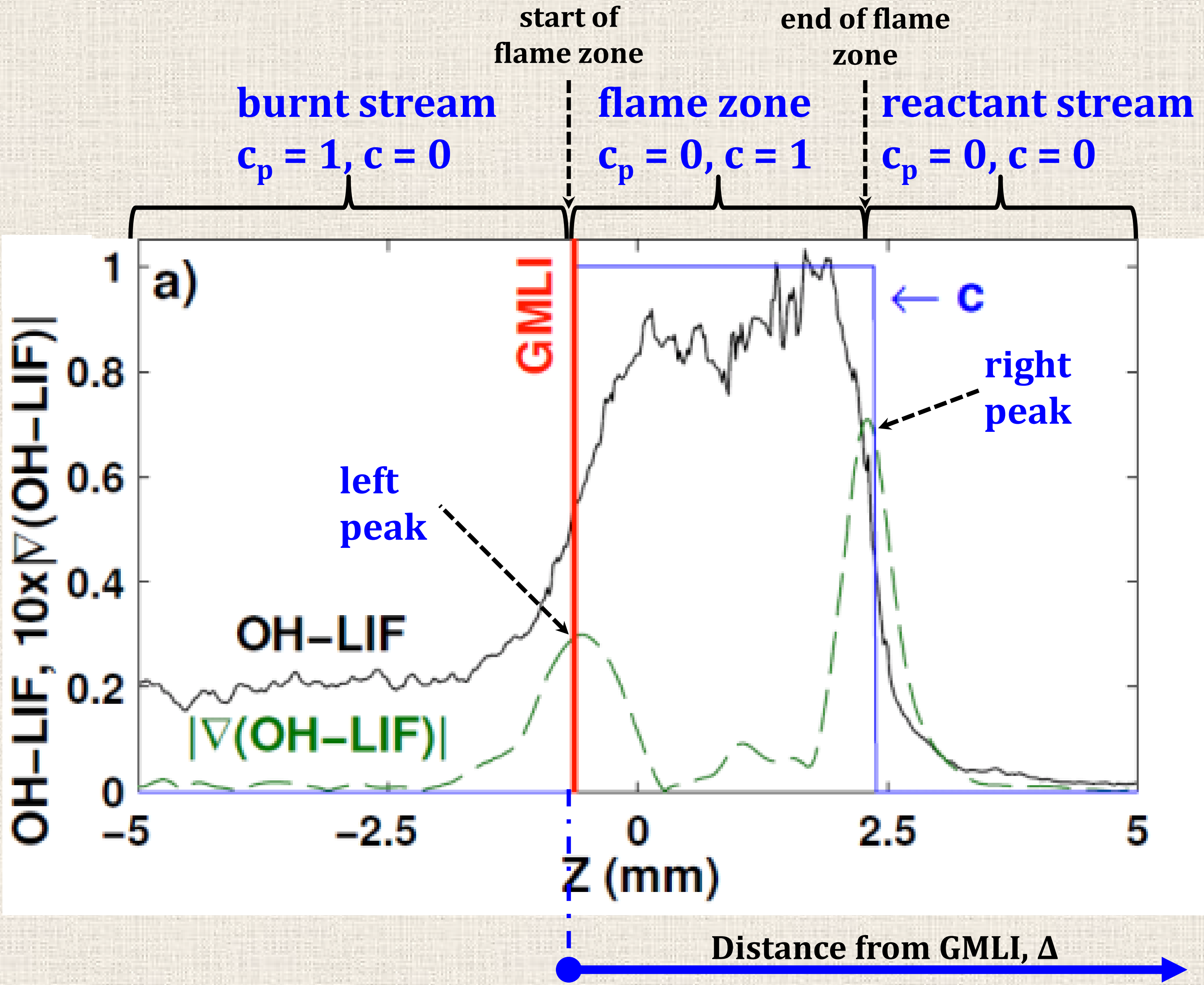


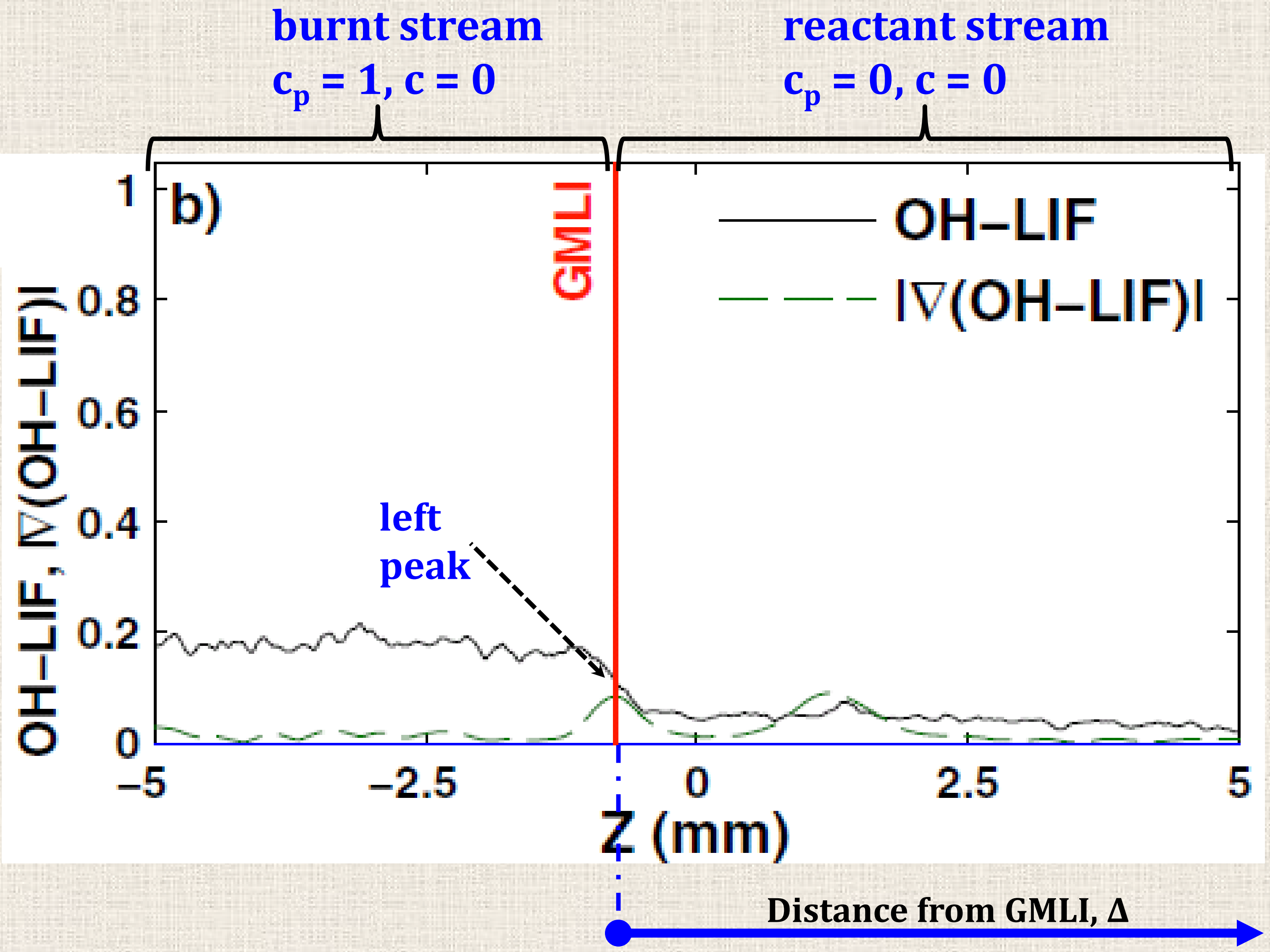

**– Simulations**

**o Experiments**

# Centerline Statistics – Progress Variable
# Intact Flame Front Contour

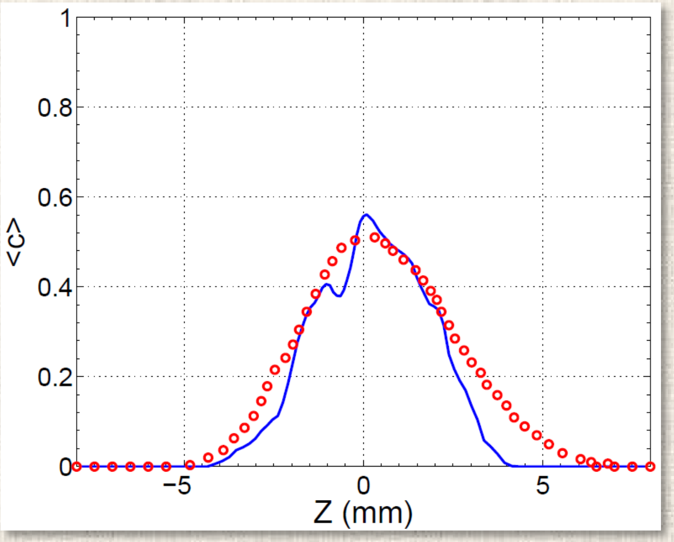


# Centerline Statistics – Progress Variable
# Local Extinction



# Cornell 4: Premixed vs. Burnt, Progress Variable

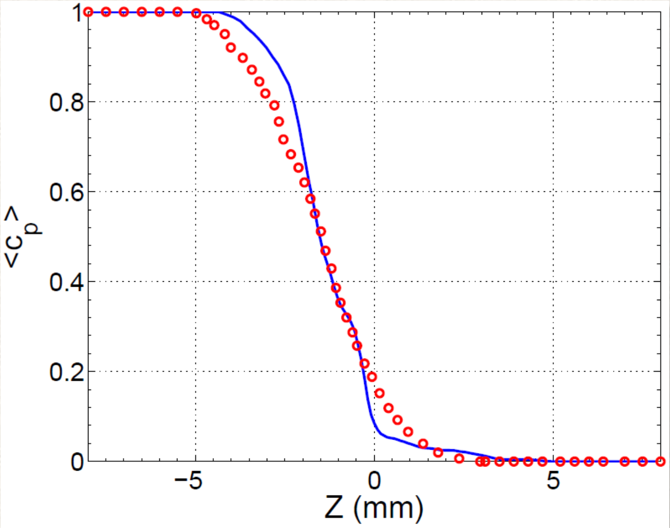
**Probability of finding turbulent flame combustion products along the burner centerline**

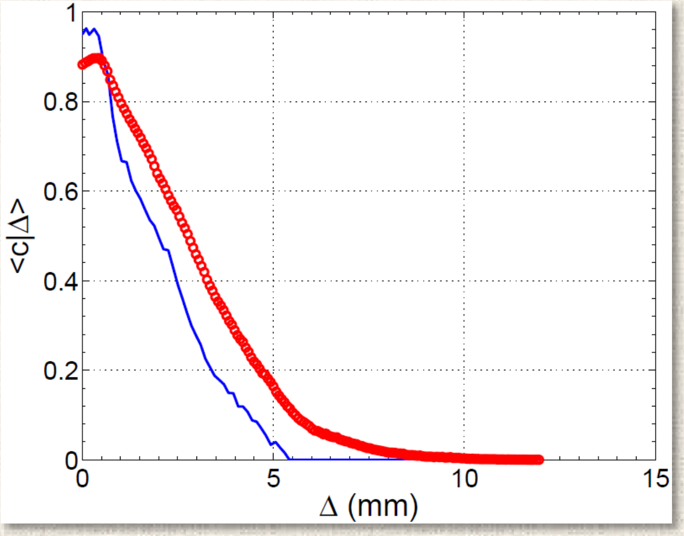



**– Simulations**

**o Experiments**

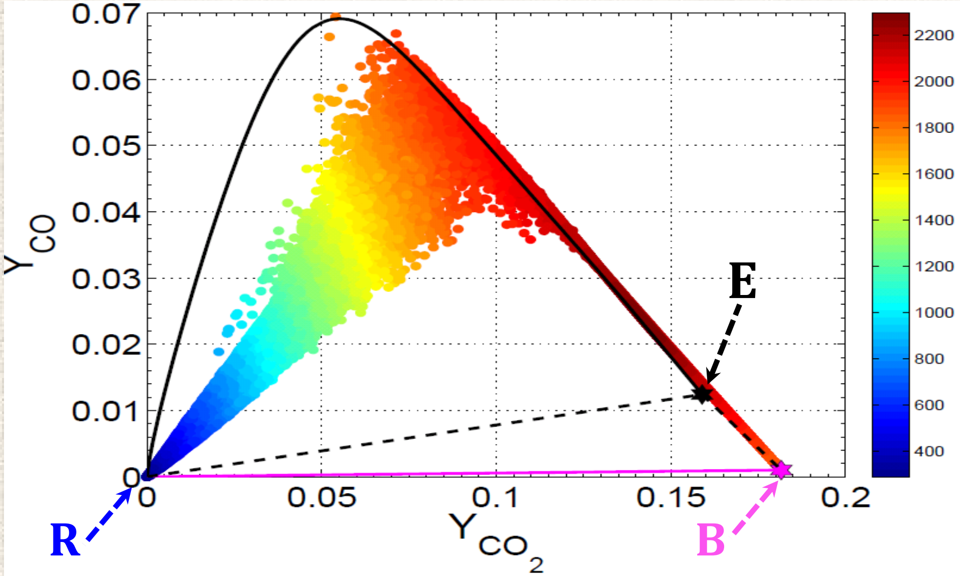
**Probability of finding counterflowing combustion products along the burner centerline**

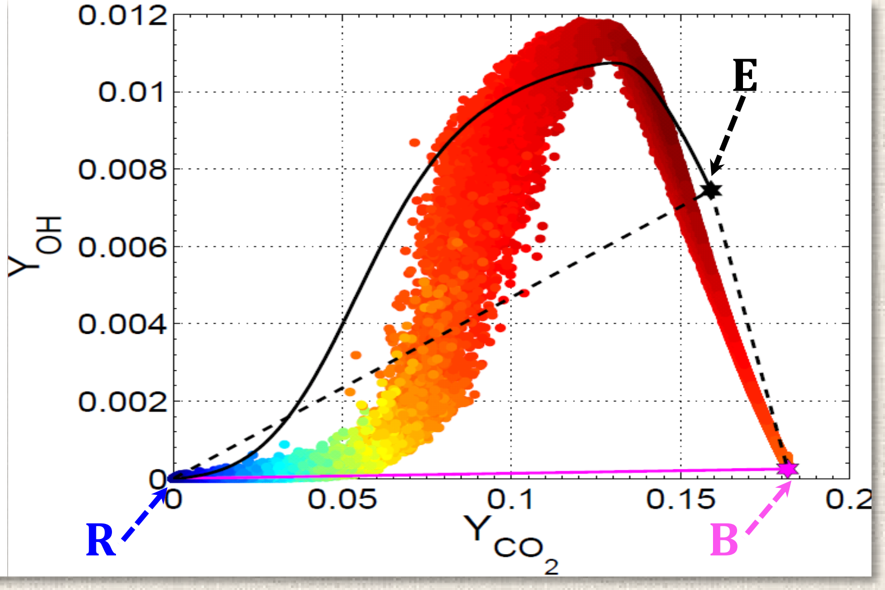



**Mean progress variable conditioned on Δ, the distance from the GMLI as a function of Δ**

# Cornell 4: Premixed vs. Burnt Scatter Plots from the HPDF Particle Data




**Reactants (R) – cold, unburnt, premixed**

**Equilibrium (E) – equilibrium composition of reactants**

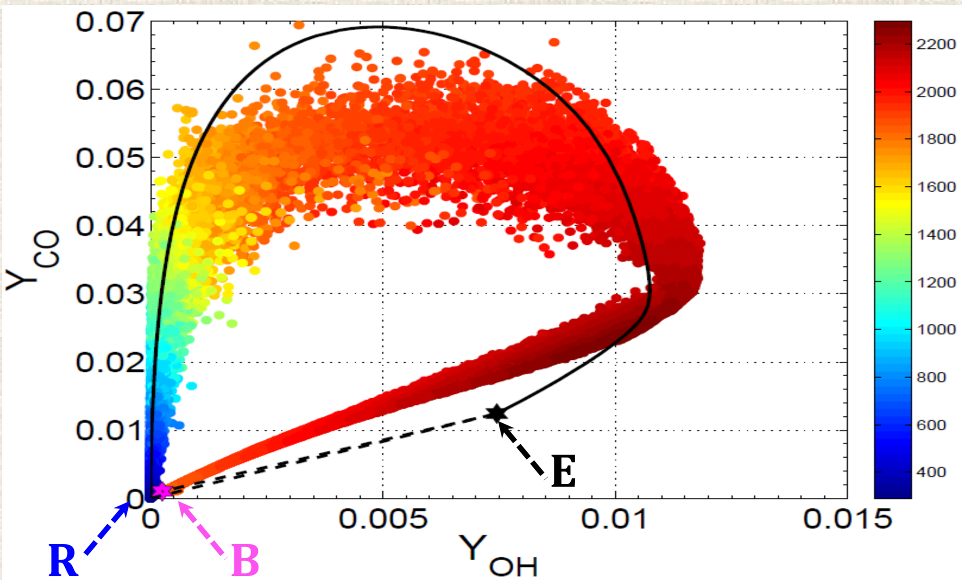
**Burnt (B) – hot products stream**

**Dots: HPDF particle data from a cylindrical region around the centerline**

**Black solid line: CHEMKIN's OPPDIF laminar solution**

**Black dash lines: Mixing line between R/E or B/E**

**Magenta solid line: Mixing line between R/B**



# CORNELL: Conclusions

- **Inflow velocity boundary conditions with TGP**
  - Scale Pettit's LES data to match experimental mean and rms near nozzle exit

- **Burnt gas nozzle (no TGP)**
  - Mean radial velocity controls location of stagnation plane
  - Significant velocity fluctuations at the exit plane

- **Generally good agreement for velocity statistics in all 4 cases**

- **Premixed vs. burnt: Good agreement with the experimental data on progress variable**
  - LES/PDF predicts a higher probability of finding flame products close to the GMLI

- **Scatter plots of species for Cornell 4, premixed vs. burnt**
  - Inert mixing between burnt stream and partially-burnt reactants
  - On reactant side, close to laminar flame solution (at high T)

# Overall Conclusions (1/2)

- Calculating the flow field and rms velocity accurately is a challenge, even when the domain includes the turbulence-generating plate
- The simpler treatments used by Brandenburg and Cornell appear satisfactory
- Specifying inflow conditions at the nozzle exits may decrease or eliminate large-scale flow instabilities
- To study turbulence-chemistry interactions, conditional statistics can be used, and these reduce the sensitivity to imperfections in the flow calculation and to large-scale flow instabilities

# Overall Conclusions (2/2)

- The LES/PDF approach (Duisberg-Essen and Cornell) appears to yields satisfactory agreement with the experimental data, including for the premixed/burnt case

- ODT appears to yield satisfactory species profiles, but it under-predicts ignition (and hence has difficulties with methane)

- More calculations are expected in the future now that groups have satisfactory flow calculations – many different experimental conditions to investigate

- It will be good to examine conditional statistics that reveal more (than mean species profiles) about the turbulence chemistry interactions