Turbulent Counterflow Flames (TCF): Modeling and Simulation

Coordinators:
Bruno Coriton
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## TNF12: TCF Modeling and Simulation Contributions

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


## Major Issue: Solution Domain and Inflow Velocity Boundary Conditions

<table>
<thead>
<tr>
<th>Group</th>
<th>Domain boundaries</th>
<th>Inflow 1</th>
<th>Inflow 2</th>
<th>Cells</th>
<th>Part.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Brandenburg</td>
<td>a) Nozzle exit planes</td>
<td>Passot-Pouquet spectrum</td>
<td>Laminar</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>CRAFT Tech.</td>
<td>b) Upstream of TGP</td>
<td>Uniform</td>
<td>Uniform</td>
<td>1.7/6m</td>
<td>-</td>
</tr>
<tr>
<td>Duisburg-Essen</td>
<td>a) and c) Downstream planes of TGPs</td>
<td>Uniform</td>
<td>Uniform</td>
<td>1.7m</td>
<td>6m</td>
</tr>
<tr>
<td>Cornell</td>
<td>a) Nozzle exit planes</td>
<td>Scaled LES data</td>
<td>Laminar</td>
<td>0.3m</td>
<td>6m</td>
</tr>
<tr>
<td>Group</td>
<td>Target</td>
<td>Configuration</td>
<td>Stream 1</td>
<td>Stream 2</td>
<td></td>
</tr>
<tr>
<td>---------------------</td>
<td>--------------</td>
<td>---------------------</td>
<td>-----------------------------------------------</td>
<td>-----------------------------------------------</td>
<td></td>
</tr>
<tr>
<td>Brandenburg</td>
<td>Sandia DNS</td>
<td>Premixed/Burnt</td>
<td>H$_2$/air, $\phi=0.4$, 294K</td>
<td>H$_2$/air, $\phi=1.0$, 1475K</td>
<td></td>
</tr>
<tr>
<td>CRAFT Tech. 1</td>
<td>Sandia/Yale</td>
<td>Inert/Burnt</td>
<td>N$_2$, 294K</td>
<td>CH$_4$/O$_2$/N$_2$, $\phi=1.0$, 1850K (O$_2$/N$_2$: 26/74 % mole)</td>
<td></td>
</tr>
<tr>
<td>CRAFT Tech. 2</td>
<td>Sandia/Yale</td>
<td>Premixed/Burnt</td>
<td>CH$_4$/O$_2$/N$_2$, $\phi=0.85$, 294K (O$_2$/N$_2$: 30/70 % mole)</td>
<td>CH$_4$/O$_2$/N$_2$, $\phi=1.0$, 1850K (O$_2$/N$_2$: 26/74 % mole)</td>
<td></td>
</tr>
<tr>
<td>Duisburg-Essen 1</td>
<td>Darmstadt</td>
<td>Fuel/Air</td>
<td>CH$_4$/air, $\phi=2.0$, 300K</td>
<td>Air, 300K</td>
<td></td>
</tr>
<tr>
<td>Duisburg-Essen 2</td>
<td>Imperial College</td>
<td>Premixed/Premixed</td>
<td>CH$_4$/air, $\phi=0.9$, 300K</td>
<td>CH$_4$/air, $\phi=0.9$, 300K</td>
<td></td>
</tr>
<tr>
<td>Cornell 1</td>
<td>Sandia/Yale</td>
<td>Inert/Inert (cold)</td>
<td>N$_2$, 294K</td>
<td>N$_2$, 294K</td>
<td></td>
</tr>
<tr>
<td>Cornell 2</td>
<td>Sandia/Yale</td>
<td>Fuel/Oxidant</td>
<td>CH$_4$/N$_2$, 294K (35/65 % mole)</td>
<td>O$_2$, 294K</td>
<td></td>
</tr>
<tr>
<td>Cornell 3</td>
<td>Sandia/Yale</td>
<td>Inert/Burnt</td>
<td>N$_2$, 294K</td>
<td>CH$_4$/O$_2$/N$_2$, $\phi=1.0$, 1850K (O$_2$/N$_2$: 26/74 % mole)</td>
<td></td>
</tr>
<tr>
<td>Cornell 4</td>
<td>Sandia/Yale</td>
<td>Premixed/Burnt</td>
<td>CH$_4$/O$_2$/N$_2$, $\phi=0.85$, 294K (O$_2$/N$_2$: 30/70 % mole)</td>
<td>CH$_4$/O$_2$/N$_2$, $\phi=1.0$, 1850K (O$_2$/N$_2$: 26/74 % mole)</td>
<td></td>
</tr>
</tbody>
</table>
ODT Modeling of a Counterflow Flame Under Intense Turbulence and Strain with Comparison to DNS

Z. Jozefik\textsuperscript{1}, A. R. Kerstein\textsuperscript{2}, and H. Schmidt\textsuperscript{1}

\textsuperscript{1}Brandenburg Technical University Cottbus-Senftenberg, Germany
\textsuperscript{2}Consultant, Danville, CA, USA

DNS results by

S. Lyra\textsuperscript{3}, H. Kolla\textsuperscript{3}, and J. H. Chen\textsuperscript{3}

\textsuperscript{3}Combustion Research Facility, Sandia National Laboratories, Livermore, CA, USA
Flow field characteristics:

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

Reactant stream turbulent inlet conditions:

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

- **Characteristic values are:**
  - $L' = 3.6 \text{ mm}$
  - $u' = 5.1 \text{ m/s}$
### Formulation:
- ODT – one-dimensional turbulence
- 1D
- Lagrangian formulation
- Variable density zero-Mach-number equations

### 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

### Empirical Input:
- ODT viscous penalty parameter $Z$
- ODT eddy frequency parameter $C$
- Maximum eddy size allowed is $5 \text{ mm} = 1.4L'$
- Stagnation point location for advection model

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

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**ODT modeling of a counterflow flame with comparison to DNS**
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

ODT modeling of a counterflow flame with comparison to DNS
Results: Favre Averaged Mean and RMS Profiles of Major Species

ODT modeling of a counterflow flame with comparison to DNS
Results: Favre Averaged Mean and RMS Profiles of Minor Species
1) ODT is able to capture the range of results shown by DNS.

ODT modeling of a counterflow flame with comparison to DNS.
Results: Statistics Conditioned on Temperature

ODT modeling of a counterflow flame with comparison to DNS
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.

ODT modeling of a counterflow flame with comparison to DNS
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
- 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 $CH_4/O_2/N_2$, $\phi = 0.85$ 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)

\[
 u_T = f (Re_T, Ka_T, a_{LES})
\]
- 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\textsubscript{2} vs. Burnt
Animation of Velocity and Product
The Stagnation Interface (SI) and Gas Mixing Layer (GMLI) interface move up and **down** between the upper and lower nozzles.
Stagnation Interface (SI) and Gas Mixing Layer (GMLI) interface move up and down between nozzles. Reduced level of the inflow turbulence at the upper nozzle is observed when the SI/GMLI is up.
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
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.
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.
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.
✓ 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
Typical instantaneous axial velocity and species contours after about 11 flow through times. N\textsubscript{2} contours are shown in black.

A simple algebraic Pocheau model is used for the turbulent flame speed.
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
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.
LES/FDF of IC Methane Premixed vs. Premixed

M. Rieth\textsuperscript{1}, F. Proch\textsuperscript{1}, A. Kempf\textsuperscript{1}
J.-Y. Chen\textsuperscript{2}, Peter Lindstedt\textsuperscript{3}

\textsuperscript{1}University of Duisburg-Essen
\textsuperscript{2}University of California Berkeley
\textsuperscript{3}Imperial College London
# Turbulent Opposed Jet Experiments and the Simulations by the Kempf Group

<table>
<thead>
<tr>
<th>Experiments</th>
<th>Simulations, Kempf group</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Imperial TOJ 1, D=25mm, Re$_{\text{max,CH}_4}$=2450(?)</strong>&lt;br&gt;Hotwire, thermocouples, mixing, scalar dissip.</td>
<td><strong>Development of combustion LES – Imperial TOJ1</strong>&lt;br&gt;Equilibrium chemistry&lt;br&gt;flowsi, 0.5 M cell, 1 CPU</td>
</tr>
<tr>
<td><strong>Darmstadt TOJ, D=30mm, Re$_{\text{max,CH}_4/\text{air}}$=7200</strong>&lt;br&gt;Line Raman-Rayleigh for scalar dissipation,&lt;br&gt;&quot;german engineering&quot;, high speed PIV</td>
<td><strong>Application of combustion LES – Darmstadt TOJ</strong>&lt;br&gt;Flamelet chemistry, pressure coupling&lt;br&gt;flowsi, 3 M cell, 1 CPU</td>
</tr>
<tr>
<td><strong>Yale TOJ, D=12.7mm, Re$_{\text{max,CH}_4/\text{air}}$=8000(?)</strong>&lt;br&gt;Bloom mixer in a plenum</td>
<td><strong>Details of in-nozzle flow – Darmstadt TOJ</strong>&lt;br&gt;Turbulence generation, jet interaction&lt;br&gt;PsiPhi, 40 M cells</td>
</tr>
<tr>
<td><strong>Imperial TOJ 2, D=30mm, Re$_{\text{CH}_4/\text{air}}$=7500</strong>&lt;br&gt;Fractal plates on Darmstadt burner Premixed &amp; against hot coflow</td>
<td><strong>Flow and combustion in new burner – Yale TOJ</strong>&lt;br&gt;PsiPhi, up to 70 M cells</td>
</tr>
<tr>
<td><strong>Development of hybrid Flamelet/FDF method in Darmstadt TOJ</strong>&lt;br&gt;Combustion, non-flamelet chemistry, extinction&lt;br&gt;PsiPhi, 1.7 M cells, 5 M particles, 4-step chemistry</td>
<td><strong>Premixed flame in Imperial TOJ2</strong>&lt;br&gt;Fractal plate generated turbulence, premixed (&amp; products)&lt;br&gt;PsiPhi, 1.7 M cells, 8 M particles</td>
</tr>
<tr>
<td>Rieth, Chen, Proch, Kempf, 2013/2014, to be submitted</td>
<td><em>Rieth, Chen, Proch, Lindstedt, Kempf, work in progress</em></td>
</tr>
</tbody>
</table>
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 ($Re_t=\sim90, U_b=3.4 \text{ m/s}$)
  - Measurements used for comparison:
    - Velocity statistics (PIV)
    - Temperature (Raman/Rayleigh)
  - Simulation contains flow between perforated plates
  - Methane with $\phi=2.0$ simulated
Imperial TOJ (Goh, Geipel, Lindstedt 2014)

- Lean premixed turbulent opposed jet flame
- Nozzle 1&2: methane, ethylene, propane (ϕ=0.7, 0.8, 0.9)
- Fractal grid generated turbulence (Reₜ=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 ϕ=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: 130x40x40mm³
- 1.7x10⁶ cells of 0.5mm³, 6x10⁶ 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)
Axial velocity (U), progress variable (C)

- Domain size: 130x40x40mm³
- 1.7x10⁶ cells of 0.5mm³, 6x10⁶ 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
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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Affiliations:
aCornell University
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cYale University
Overview

- **Simulation approach**
  - LES-PDF methodology

- **Simulations of Yale burner**
  - Cornell 1: Isothermal flow – N₂ vs. N₂
  - Cornell 2: Non-premixed flame – CH₄/N₂ vs. O₂
  - Cornell 3: Inert/Burnt – N₂ vs. Hot product stream
  - Cornell 4: Premixed/Burnt – CH₄/O₂/N₂ 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 (Φ) 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

Temperature  \( Y_{CO_2} \)  \( Y_{OH} \)  \( Y_{N_2} \)

TPDF  YCO2PDF  YOHPDF  YN2PDF
2326  0.18  1.20e-02  1.00
1818  0.14  8.97e-03  0.91
1310  0.09  5.98e-03  0.81
802   0.05  2.99e-03  0.72
293   0.00  0.00e+00  0.63
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

\[ U_{i,\text{React}}(r, \theta, t) = \left< U_i(r) \right>_{\text{exp,React}} + \alpha_i(r) \left[ U_{i,\text{nozzle}}(r, \theta, \beta t) - \left< U_i(r) \right>_{\text{nozzle}} \right] \]

- **Notation:**
  - \( \alpha_i(r) \): to match the r.m.s velocity; \( \beta = T_{\text{nozzle}}/T_{\text{React}} \): to match the turbulent length scale/time scale;
  - \( U_{i,\text{nozzle}} \) is Pettit’s nozzle simulation velocity time-series data;
  - \( \left< U_i(r) \right>_{\text{exp,React}} \) is the velocity mean from experiments available at 0.5 mm downstream of the nozzle exit;
  - \( U_{i,\text{React}} \) 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 \( \left< U \right> \) is scaled to achieve the required volume flow rate
- Radial velocity profile \( \left< V \right> \) 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

- Experiments
- Simulations
- Pettit et al.
Cornell 2: Non-Premixed Centerline Velocity and OH

- Simulations
- Experiments

\[
\frac{\langle U \rangle}{U_{\text{bulk}}} \quad \text{and} \quad \frac{U'}{U_{\text{max}}} \quad \text{versus} \quad z \quad \text{(mm)}
\]
Cornell 3: $N_2$ vs. Burnt
Centerline Velocity Mean and RMS

- Simulations
- Experiments
Cornell 4: Premixed vs. Burnt Centerline Velocity Mean and RMS

- Simulations
- o Experiments
Centerline Statistics – Progress Variable
Intact Flame Front Contour

- burnt stream: $c_p = 1, c = 0$
- flame zone: $c_p = 0, c = 1$
- reactant stream: $c_p = 0, c = 0$

Distance from GMLI, $\Delta$
Centerline Statistics – Progress Variable
Local Extinction

burnt stream
$c_p = 1, c = 0$

reactant stream
$c_p = 0, c = 0$

Distance from GMLI, $\Delta$
Simulations and experiments show the probability of finding turbulent flame combustion products and counterflowing combustion products along the burner centerline.

Mean progress variable conditioned on $\Delta$, the distance from the GMLI as a function of $\Delta$.
**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 OPPDIFF laminar solution

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

Magenta solid line: Mixing line between R/B
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)
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.