Effects of Exhaust Gas Recirculation (EGR) on Turbulent Combustion and Emissions in Advanced Gas Turbine Combustors with High-Hydrogen-Content (HHC) Fuels

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LES Modeling

- Overarching Objective
  - Development of a predictive, integrated Large Eddy Simulation (LES) model for turbulent premixed flame structure and NOx emissions in the presence of carbon dioxide and water dilution [at elevated pressure]

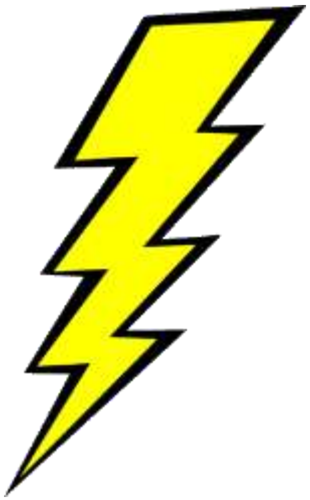
- Today's Questions
  - What matters?
  - When does it matter?
  - Why does it matter?

LES Modeling

- LES Model Development/Analysis
  - Heat Loss Modeling with Low-Dimensional Manifolds
  - Sensitivity Analysis
    - Manifold Construction
    - Chemical Mechanism
- RATS Burner Simulations
- PARAT Burner Simulations

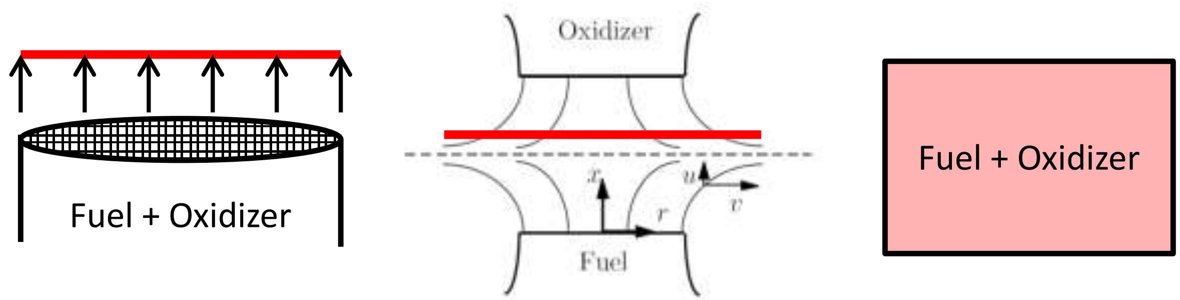
Model Development

- Fundamental Turbulent Combustion Challenge
  - Too many species (computational cost)
  - Closure too difficult (human cost)



Model Development

- Physically-Derived Reduced-Order Manifolds (PDROM)
  - Approximate turbulent combustion processes with component model problem (real or imagined)



  - Parameterize model problem solutions with a smaller number of variables (low-dimensional manifold)

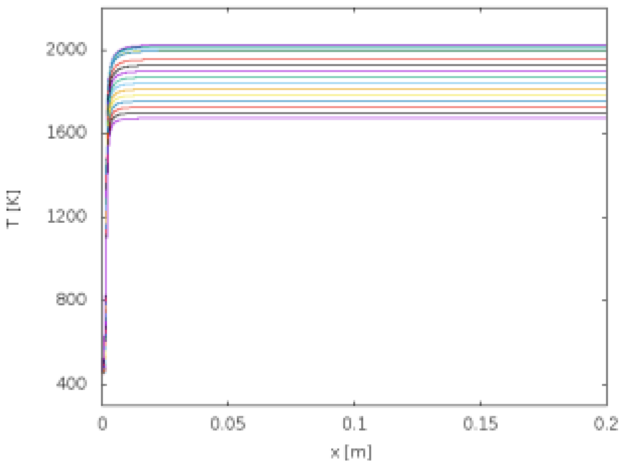
$$Y_k = g(Z, C, \ldots)$$

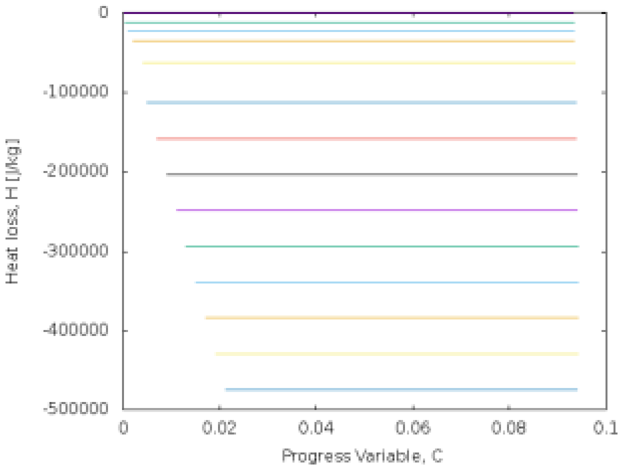
Model Development

- Premixed Combustion with PDROM
  - Component Problem: Unstretched premixed flames
  - Governing Equations: $\rho_u S_L^0 \frac{dY_k}{dx} = \frac{d}{dx}\left(\rho D \frac{dY_k}{dx}\right) + \dot{m}_k$
    - Solve equations at multiple mixture fractions
    - More convenient than equations in progress variable space
  - Parameterizing Variables
    - Progress Variable, $C = Y_{H_2} + Y_{H_2O}$
    - Mixture Fraction, Z
  - (Note: Only NO production rate taken from manifold.)
  - How to consider radiation heat losses?
    - Critical for predictions of nitrogen oxides

Model Development

- Heat Losses: Approach I[1]
  - Add enthalpy deficit H as additional parameterizing variable
    - Defined to be zero for adiabatic
  - Solve premixed flames with varying unburned enthalpy
    - "Cold Boundary" Problem: Convert fuel/air to products rather than decreasing the unburned temperature





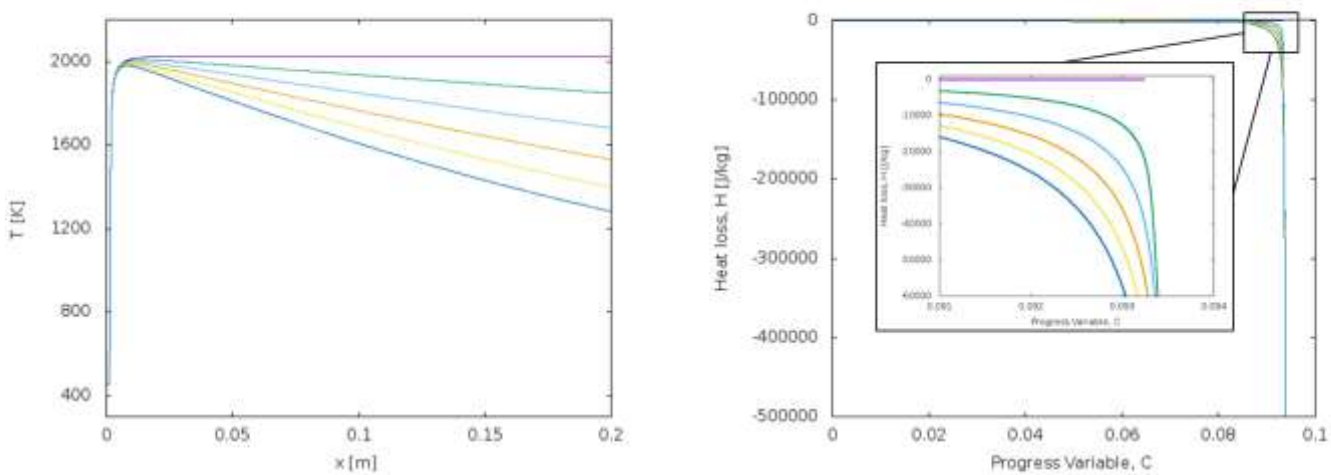
- Hypothesis: Product conversion masks EGR chemical effects

[1]J.A. van Oijen, F.A. Lammers, L.P.H. de Goey, Combust. Flame 127 (2001) 2124-2134

Model Development

- Heat Losses: Approach II[1]
  - Augment premixed flame equations with equation for heat loss parameter with radiation source term and variable coefficient β:

$$\rho_u s_L \frac{dH}{dx} = \frac{d}{dx}\left(\rho D_H \frac{dH}{dx}\right) + \beta \dot{q}_{rad}$$



  - Annoyance: Less “fully accessible” manifold in C-H space

[1]A.C. Nunno, T. Grenga, M.E. Mueller, Eastern States Section Combustion Institute Spring Meeting, 2016

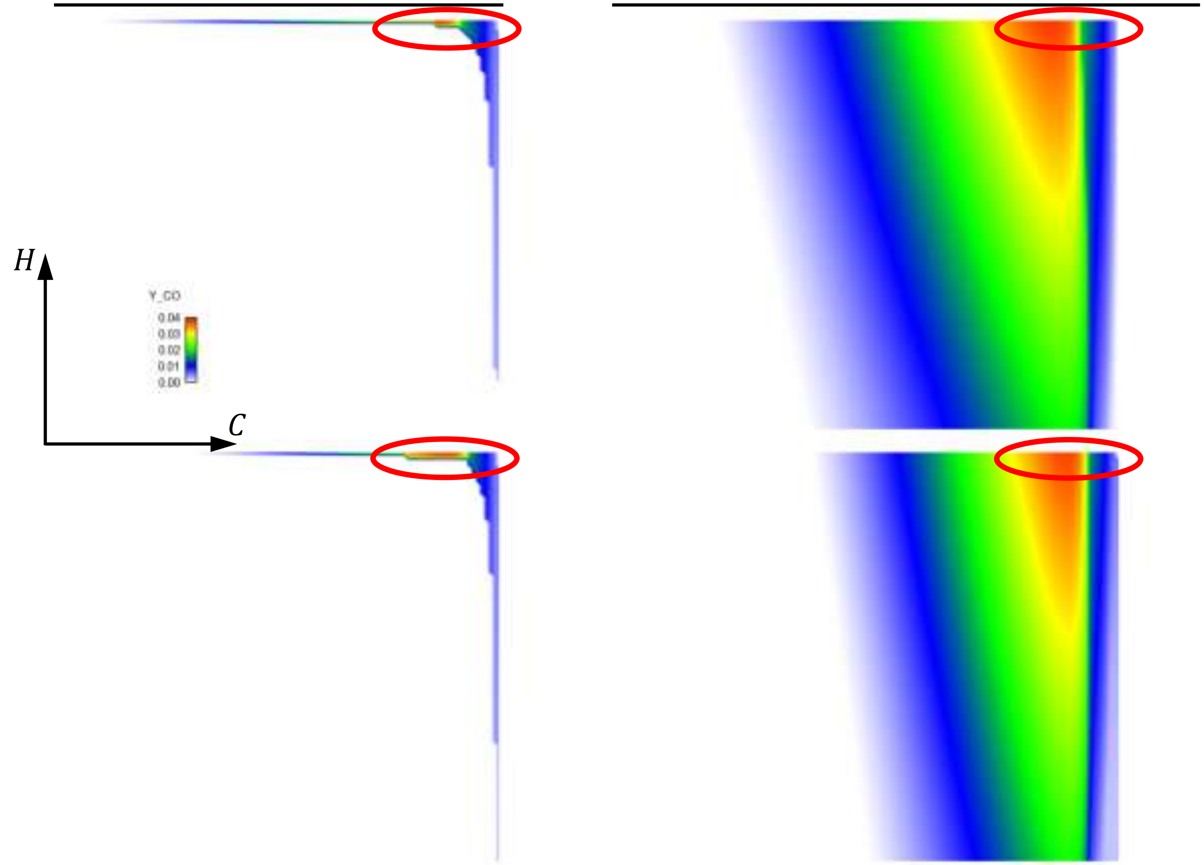
Model Analysis

- Sensitivity to Manifold Construction (CO)

"Source Term" Method | "Product Conversion" Method

Methane/Air Flame with Nitrogen Dilution:

Methane/Air Flame with Water Dilution:



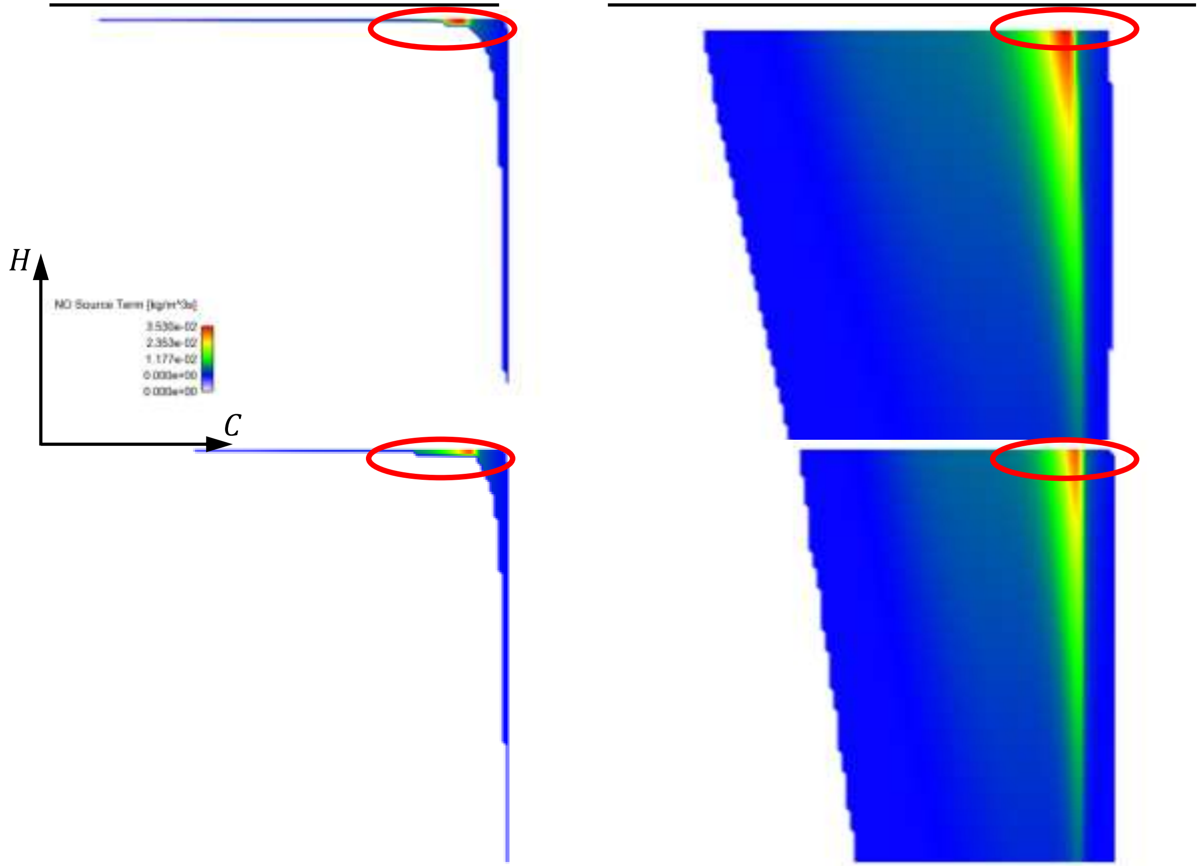
Model Analysis

- Sensitivity to Manifold Construction (NO Production Rate)

"Source Term" Method | "Product Conversion" Method

Methane/Air Flame with Nitrogen Dilution:

Methane/Air Flame with Water Dilution:

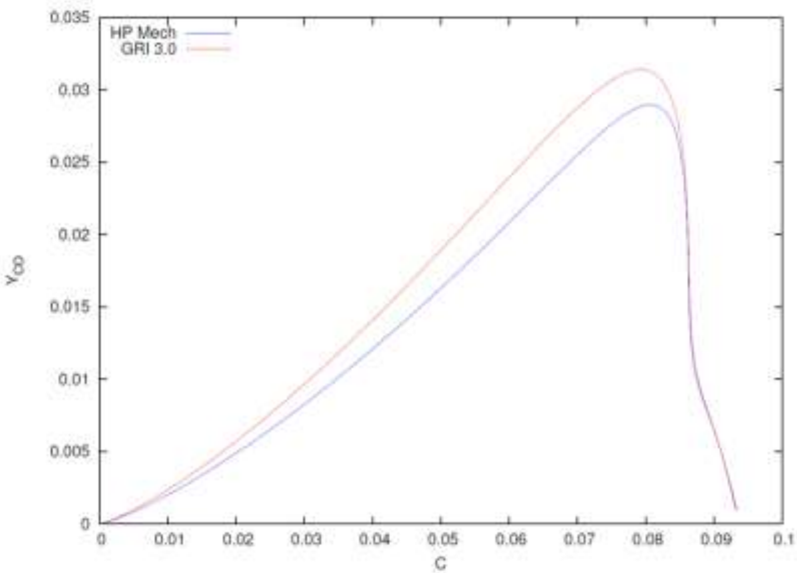


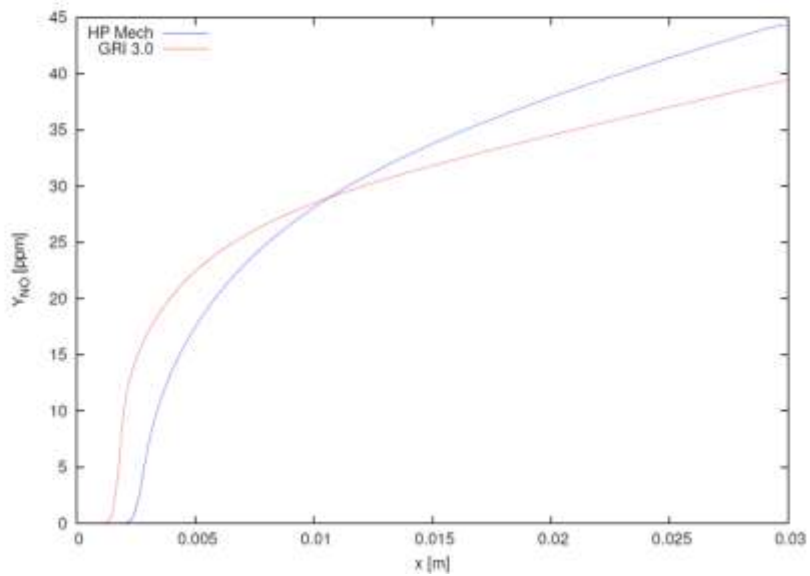
Model Analysis

- Sensitivity to Manifold Construction
  - The two manifolds are identical within plotting accuracy!
    - The only difference is the accessible region, which is controlled by the range of the source term coefficient β or variation in unburned enthalpy.
    - However, in the results shown later, β is set such that all points in the simulation appear in the accessible portion of the manifold, meaning that the "product conversion" method simply provides many unneeded states.
    - Hypothesis regarding pollution of EGR chemical effects with the production conversion method was proven false.
  - Precise details of how a manifold is generated is a secondary concern to the component model problem and parameterizing variables

Model Analysis

- Sensitivity to Chemical Mechanism
  - Same methane/air flame with nitrogen dilution

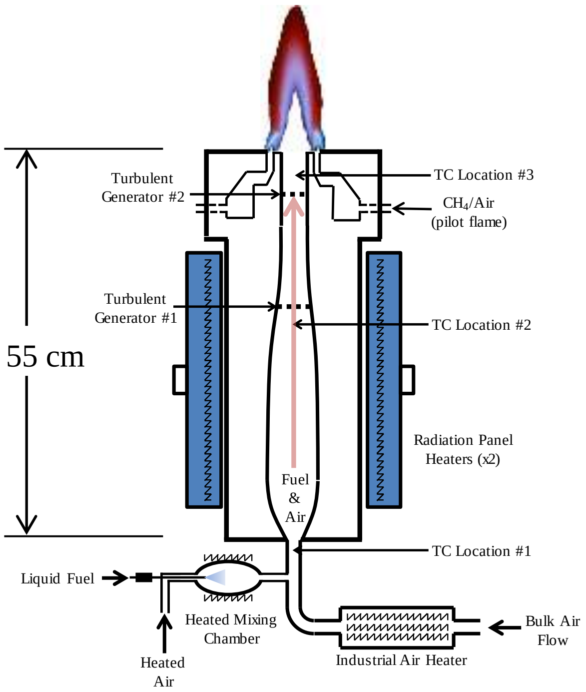




- Far greater sensitivity to underlying chemical kinetic model!

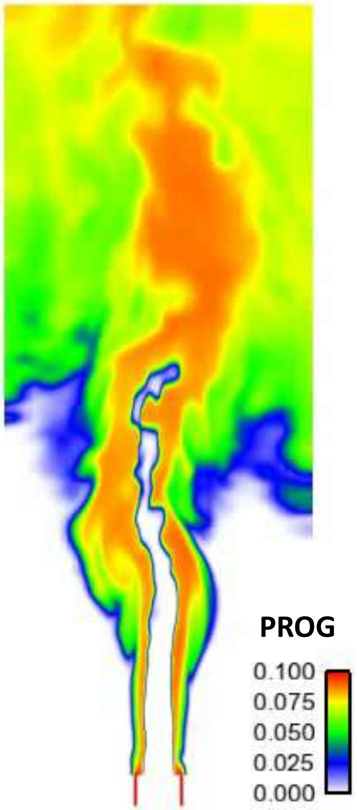
RATS Burner

- Test Conditions
  - Methane/air: $\phi = 0.9$
  - $U_{\text{jet}} = 15 \text{ m/s}$
  - $\text{Re} \approx 8{,}500$
  - H_2O/CO_2 dilution
    - 10% by volume
    - N2 dilution to maintain constant flame temperature of 2025 K
  - Pilot
    - Stoichiometric methane/air without dilution with $U_u = 1 \text{ m/s}$



RATS Burner

- Computational Infrastructure: NGA[1,2]
  - Numerical Methods and Turbulence Models
    - Space: Second-order velocity; third-order scalars
    - Time: Second-order semi-implicit
    - Dynamic Smagorinsky models for turbulent transport
  - Computational Domain
    - 1.6M grid points $(256 \times 192 \times 32)$
    - Domain length: $20H$
  - Boundary Conditions
    - Jet: Forced isotropic turbulence with matched integral scale and turbulence intensity
    - Coflow: Weak to mimic entrainment
    - Pilot: Stoichiometric mixture with consistent dilution and unburned velocity of $1\ \mathrm{m/s}$ (little sensitivity)

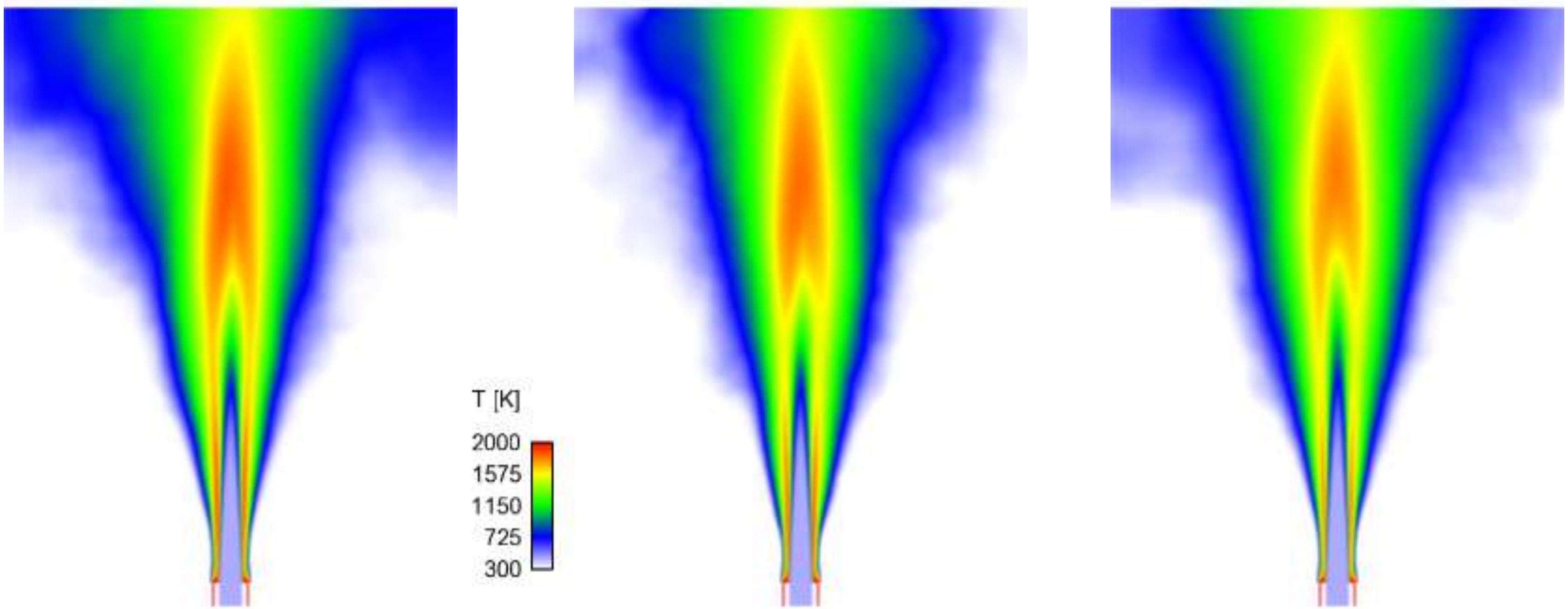


[1]O. Dejsardins, G. Blanquart, G. Balarac, H. Pitsch, J. Comp. Phys. 227 (2008) 7125-7159
[2]J.F. MacArt, M.E. Mueller, J. Comp. Phys. 326 (2016) 569-595

RATS Burner

- Results: Temperature

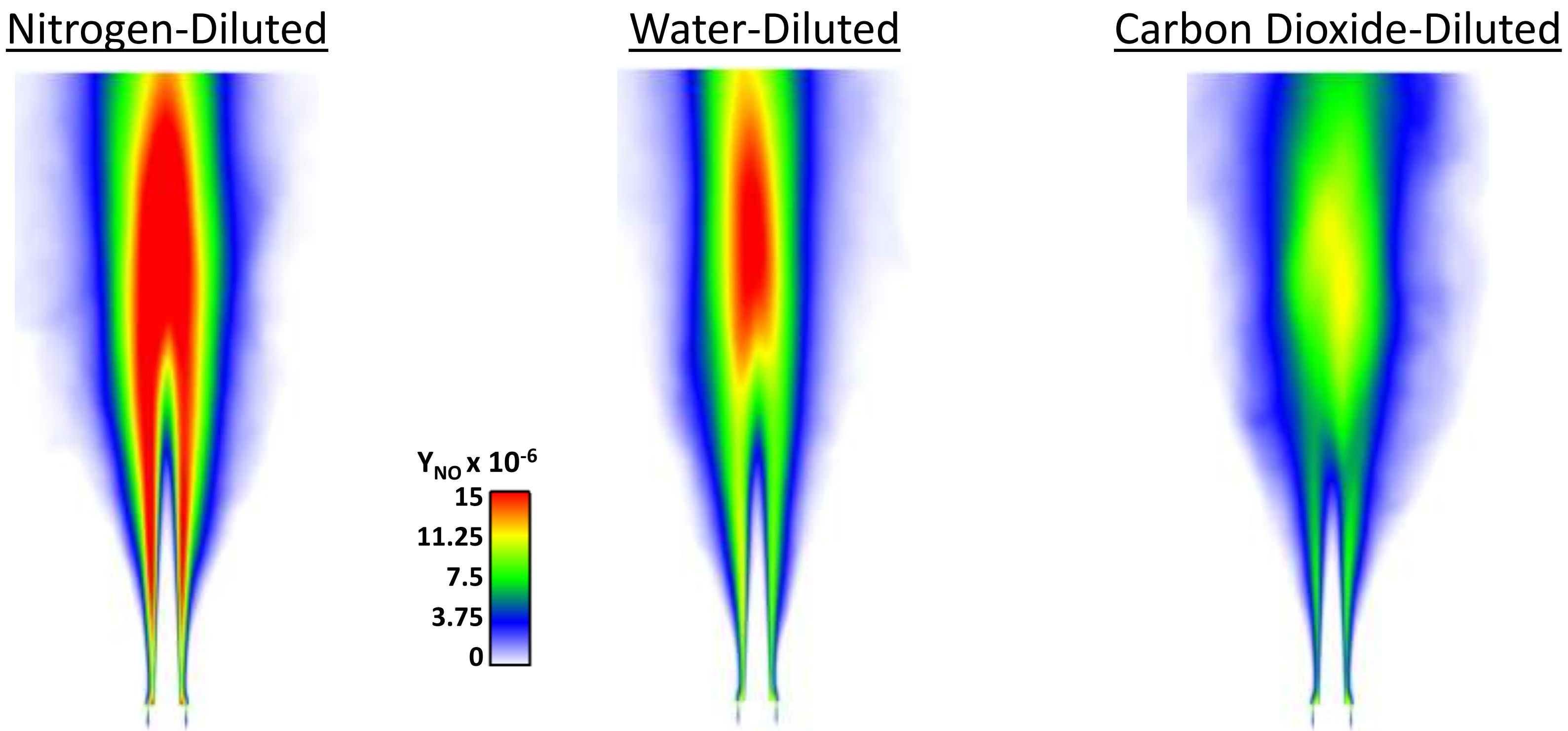
Nitrogen-Diluted | Water-Diluted | Carbon Dioxide-Diluted



  - Post-flame temperature $T_{CO2} < T_{H2O} < T_{N2}$ due to increased heat losses with diluents

RATS Burner

- Results: NO Mass Fraction



  – Decrease in post-flame NO most strongly correlated with temperature; chemical effect of H_2O addition secondary

Shift
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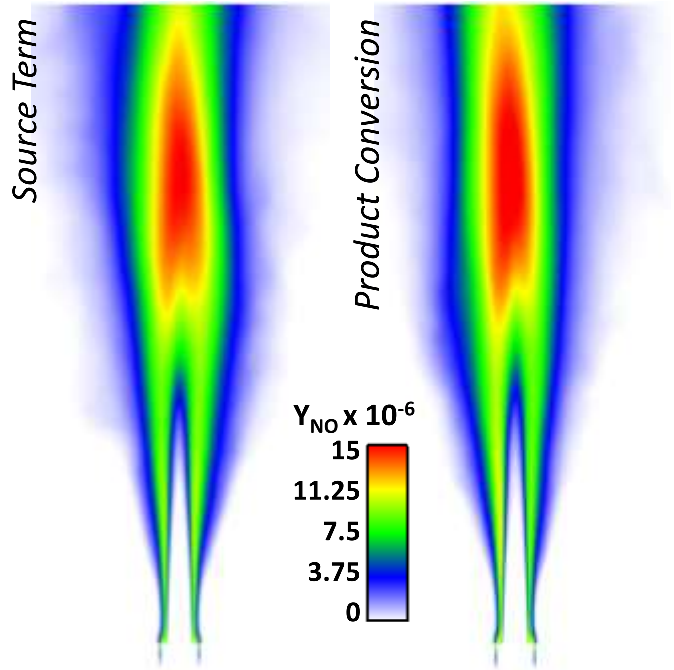
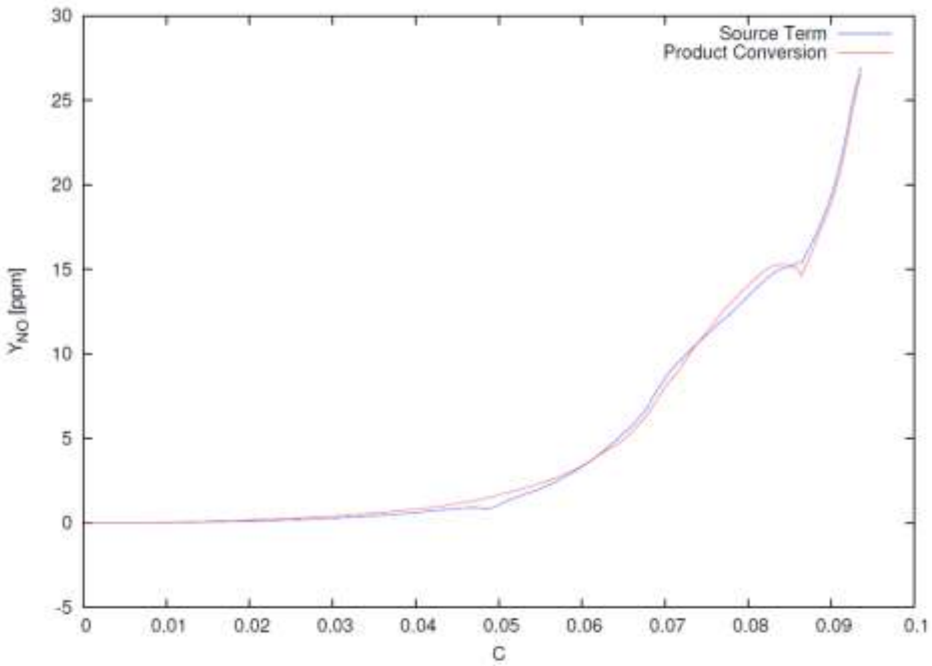
RATS Burner

- Results: Comparison of Manifold Generation

Water-Diluted



Nitrogen-Diluted



– Negligible effect of the manifold generation process

Ongoing Work: PARAT Burner

- Preliminary Reacting Flow Calculations
  - Jet Boundary Condition: Fully developed pipe flow
    - New Purdue measurements of exit velocity profile
  - Pilot Boundary Condition: Methane/air mixture rather than hydrogen/air mixture
    - Assessing sensitivity to pilot velocity with different fuel/air mixture (too much local extinction on right)
    - Under separate funding, building capability to accommodate different pilot fuel/air mixture in more general PDROM approach (many-stream systems)
  - Coflow Boundary Condition: Weak coflow instead of wall
    - Assessing to coflow velocity
  - <u>Current Effort</u>: Quantitative comparisons with Purdue experimental measurements