Oxy-Combustion Modeling for Direct-Fired sCO_2 Power Cycles

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Background and Motivation

Allam Cycle (NetPower)

- Direct-fired (Allam) cycle operates at very high pressures (300 bar) with CO_2 dilution.
- There is a lack of experimental data and modeling experience at these conditions.
- CFD is expected to play a key role in combustor design (flame holding, heat release, CO formation, etc…).
- CO has a significant impact on cycle efficiency.
- Combustion sub-models have not been validated at these conditions.

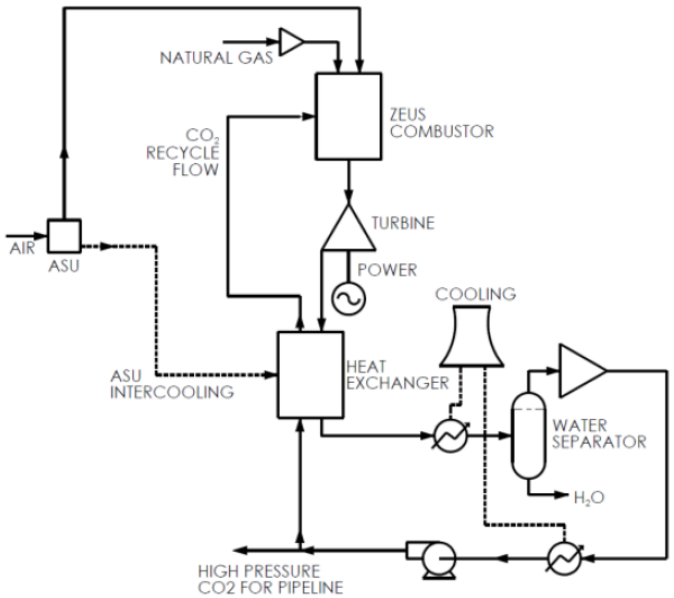


Figure 1. BASIC ALLAM CYCLE NATURAL GAS FLOW DIAGRAM.

Point	Pressure (Bar)	Temperature (°C)
Turbine Inlet (A)	300	1150
Turbine Outlet (B)	30	775
CO2 Compressor Inlet (D)	30	20
CO2 Compressor Outlet (E)	80	65
CO2 Pump Inlet (F)	80	20
CO2 Pump Outlet (G)	300	55
Combustor Inlet (I)	300	750

R.J. Allam et. al., ASME GT2014-26952, 2014   ** Allam, et al., Energy Procedia 37, 2013, 1135-1149*

Three Combustion Modeling Approaches

Three of many…

1) No Turbulence Chemistry Interaction (Laminar).

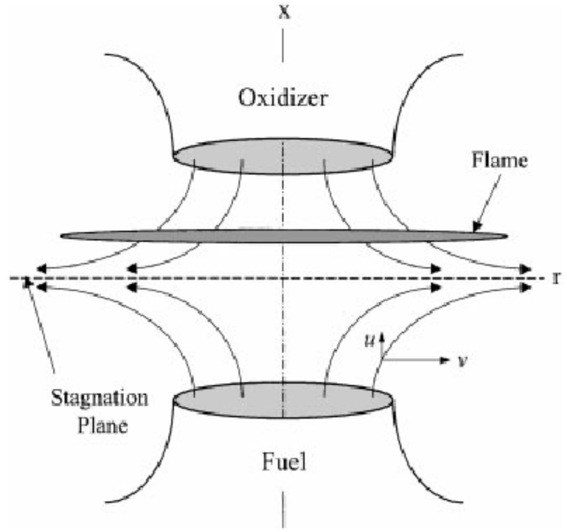
- Ignores sub-grid fluctuations in temperature and concentration.
- Similar to fast mixing at the sub-grid scale.

2) Flamelet Model.

- Assumes turbulent flame is an ensemble of strained laminar flamelets.
- Pre-tabulated table of thermodynamic properties as a function of mixture fraction and local strain rate.

3) Filtered Density Function (composition PDF transport).

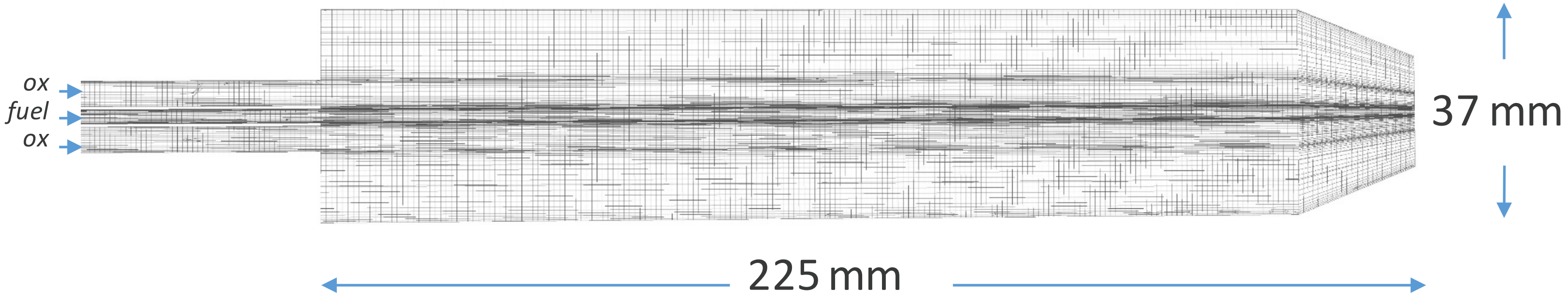
- Transport equation for single-point joint PDF solved (thermochemical state).
- Chemical source term is closed but molecular mixing must be modeled.
- Solved by Monte-Carlo methods (Lagrangian “particle” tracking).
- Coupling with flow solver through density.



$$\frac{\partial F_L}{\partial t} + \frac{\partial[\langle u_i\rangle_L F_L]}{\partial x_i} = \frac{\partial}{\partial x_i}\left[\left(\gamma + \gamma_t\right)\frac{\partial\left(\frac{F_L}{\langle\rho\rangle_l}\right)}{\partial x_i}\right] + \frac{\partial}{\partial \psi_\alpha}\left[\Omega_m(\psi_\alpha - \langle\varphi_\alpha\rangle_L)F_L\right] - \frac{\partial(S_\alpha F_L)}{\partial \psi_\alpha}$$

Computational Setup

Single Injector Domain



3D 590k hex cells
m_F = 0.04762 kg/s
Phi = 0.95
T_F = 476 K
T_O = 1014 K
P = 300 bar
2.4 MW

- Large Eddy Simulation with transported *k*-equation.
- 16 Species skeletal mechanism from UCF.*
- Incompressible, pressure-based solver. 2nd order in space and time. Max Courant # ~ 1.
- CO_2 added to oxidizer stream to change O_2 concentration.
- ANSYS Fluent V18.2

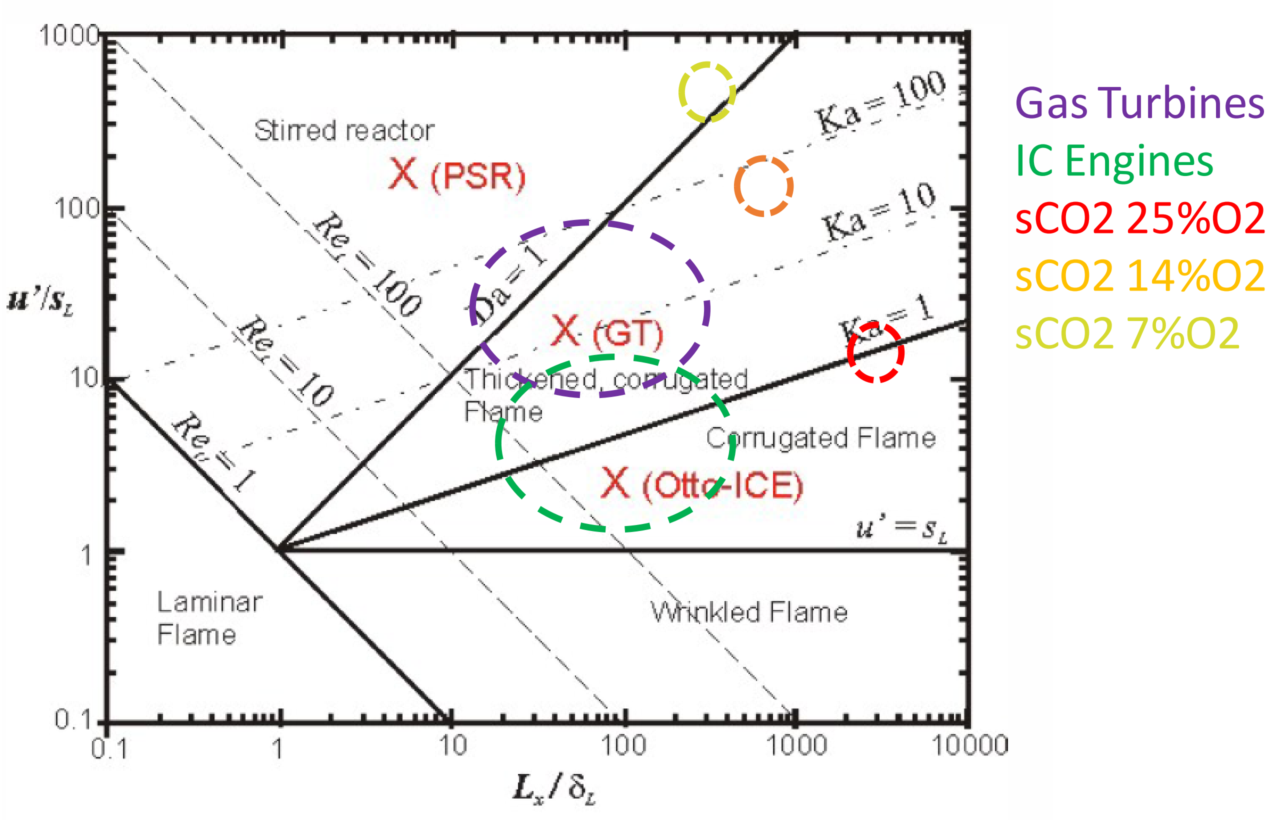
parameter	Case 1	Case 2	Case 3
O_2 mass fraction	0.250	0.138	0.070
U_{ox} (m/s)	54	94	180
l_T (m)	1.9e-3	2.2e-3	2.0e-3
U' (m/s)	7.5	10.7	23.8
S_L (m/s)	0.58	0.082	0.05
τ_{ign} (s)	1.5e-3	1.6e-3	2.0e-3

*K.R.V. Manikantachari, V. Ladislav, S. Martin, J.O. Bobren-Diaz and S. Vasu, "Reduced Chemical Kinetic Mechanisms for Oxy/Methane Supercritical CO2 Combustor Simulations", J. Energy Resources Technology-Transactions of the ASME, accepted 3/2018.

Borghi Diagram for Oxy-Combustion

- **Three cases shown for 300 bar oxy-combustion define a range of conditions (O_2 from 7-25%) spanning the thickened, corrugated flame regime and stirred reactor.**

- **Significantly outside the range of gas turbine and IC engine operation.**
  - Re# and/or Ka# significantly larger than gas turbines or IC engines.
- **Requires assessment of appropriate turbulent combustion models.**

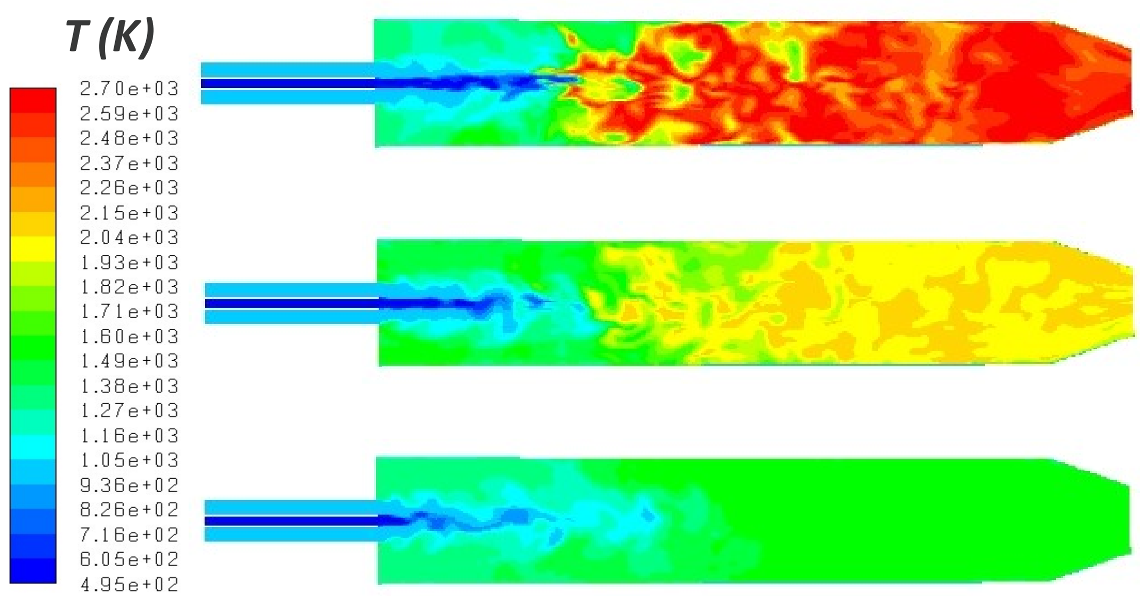


Effect of O_2 Concentration

Laminar Model

- Lifted flame at 25% O_2 transitions to autoignition reaction at 7% O_2.
- Similar behavior for both Laminar and FDF models.
- Flamelet model unable to predict autoignition behavior for 7% O_2 case.

Instantaneous Temperature (K)



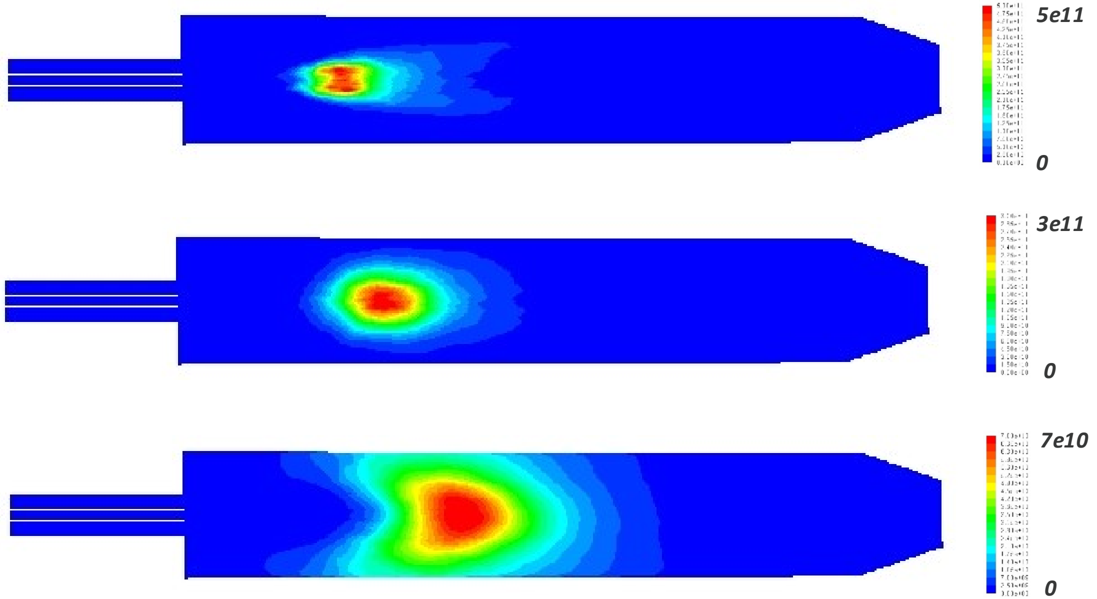
O2 mass fraction

25%

14%

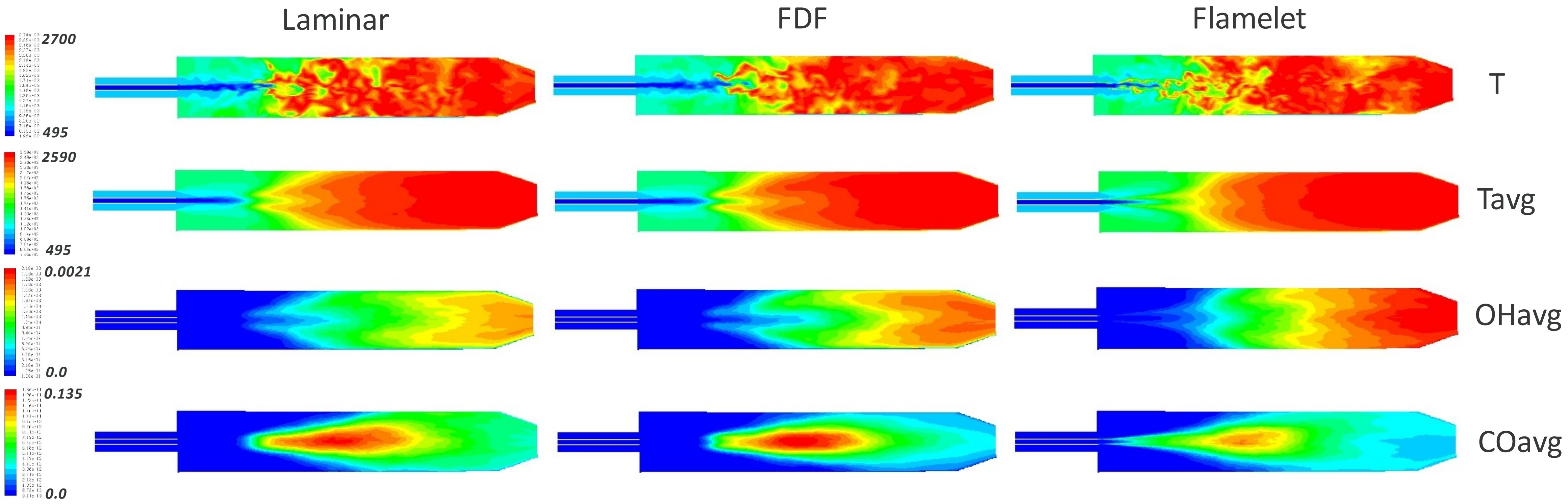
7%

Mean RR (W/m^3)



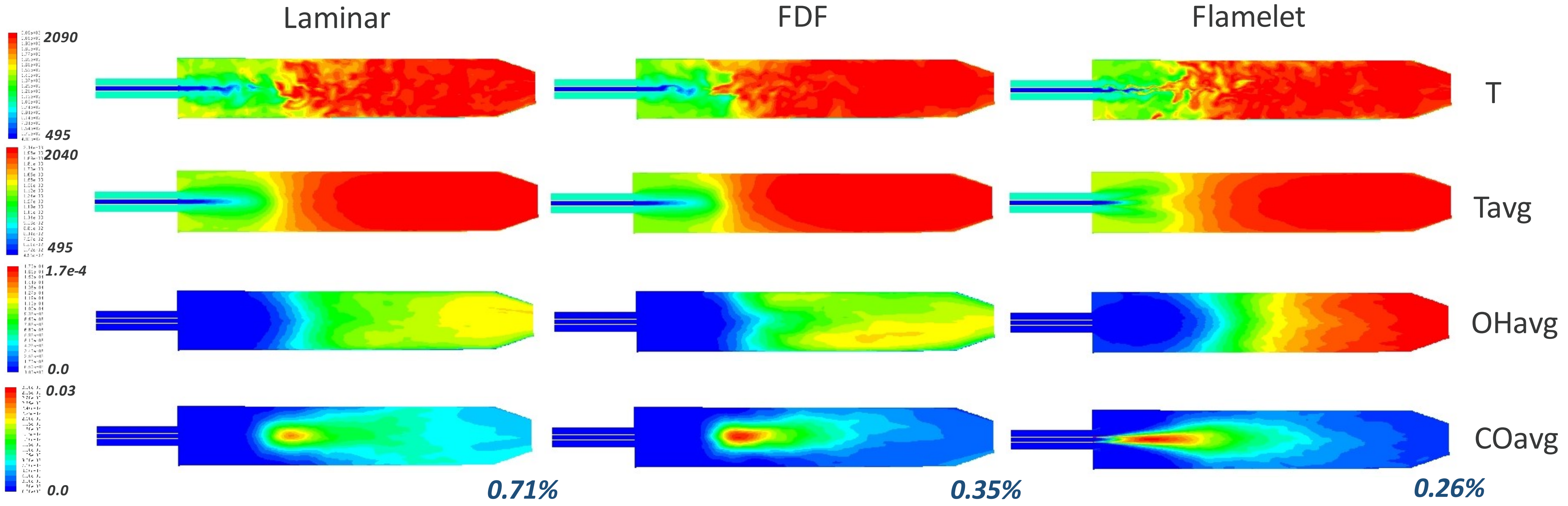
Results for Case 1 (25% O_2)

- Similar flame shape for all three models (lifted flame).
- Peak CO concentration similar for Laminar and FDF models although FDF predicted lower exit CO (3.0% vs 4.4% mass fraction). Maybe better burnout?



Results for Case 2 (14% O_2)

- Similar flame shape for Laminar and FDF models, Flamelet model predicts intermittent flame attachment to injector.
- Similar trend in CO for Laminar and FDF models (similar peak CO and better burnout for FDF model).



CO Formation and Destruction

16 Species Skeletal Mechanism*

- Main CO formation paths:

  $$HCO + M = H + CO + M$$

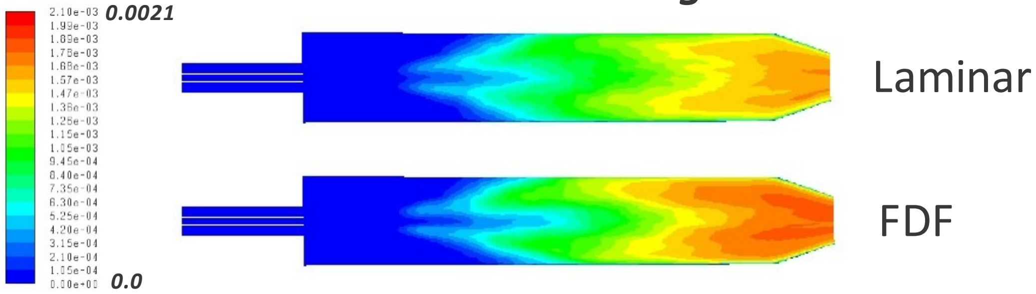
  $$HCO + O_2 = CO + HO_2$$

- Main oxidation path:

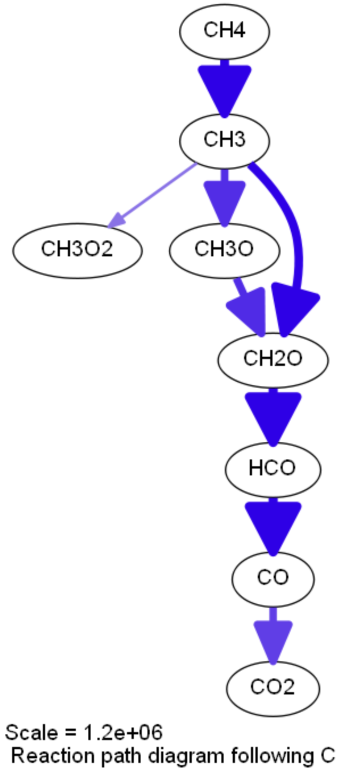
  $$CO + OH = CO_2 + H$$

- Since Laminar and FDF models show similar temperature and OH profiles, “burnout” is not likely the cause of discrepancy in exit CO.

25% O2 OH avg



Path Flux Analysis



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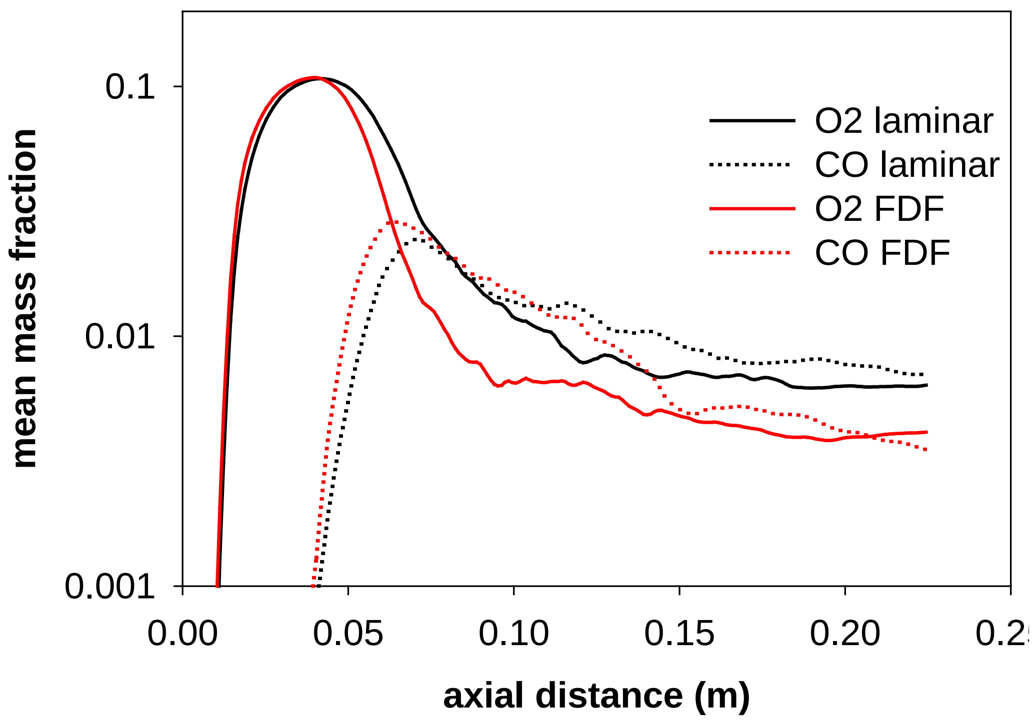
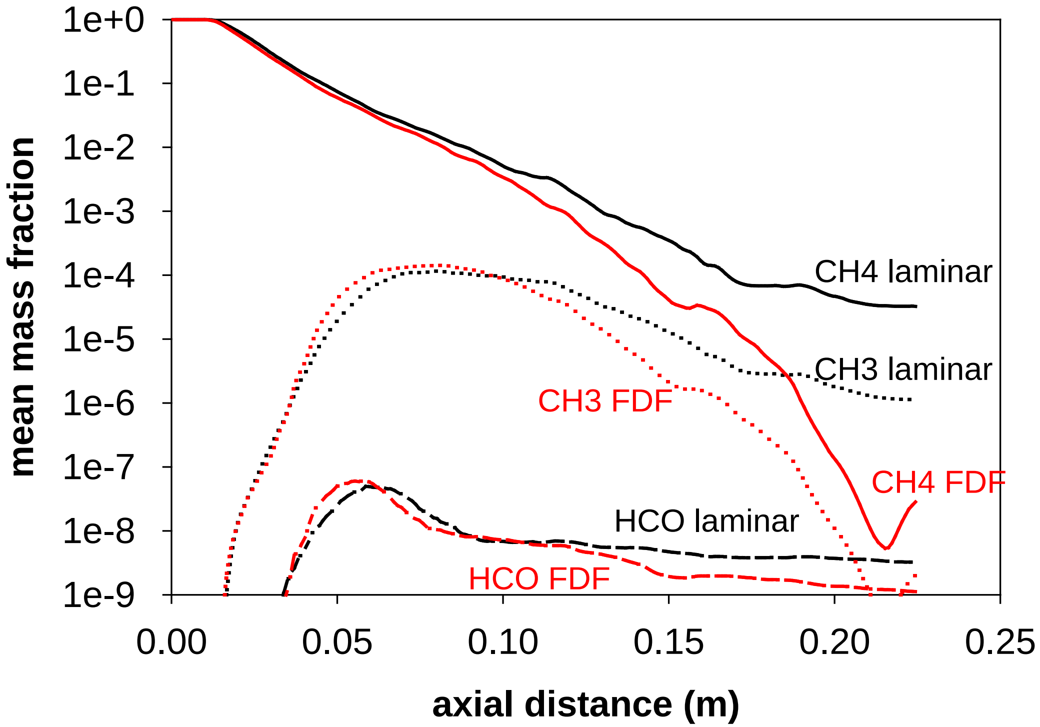
Centerline profiles for Case 2 (14% O_2)

Mean Mass Fractions



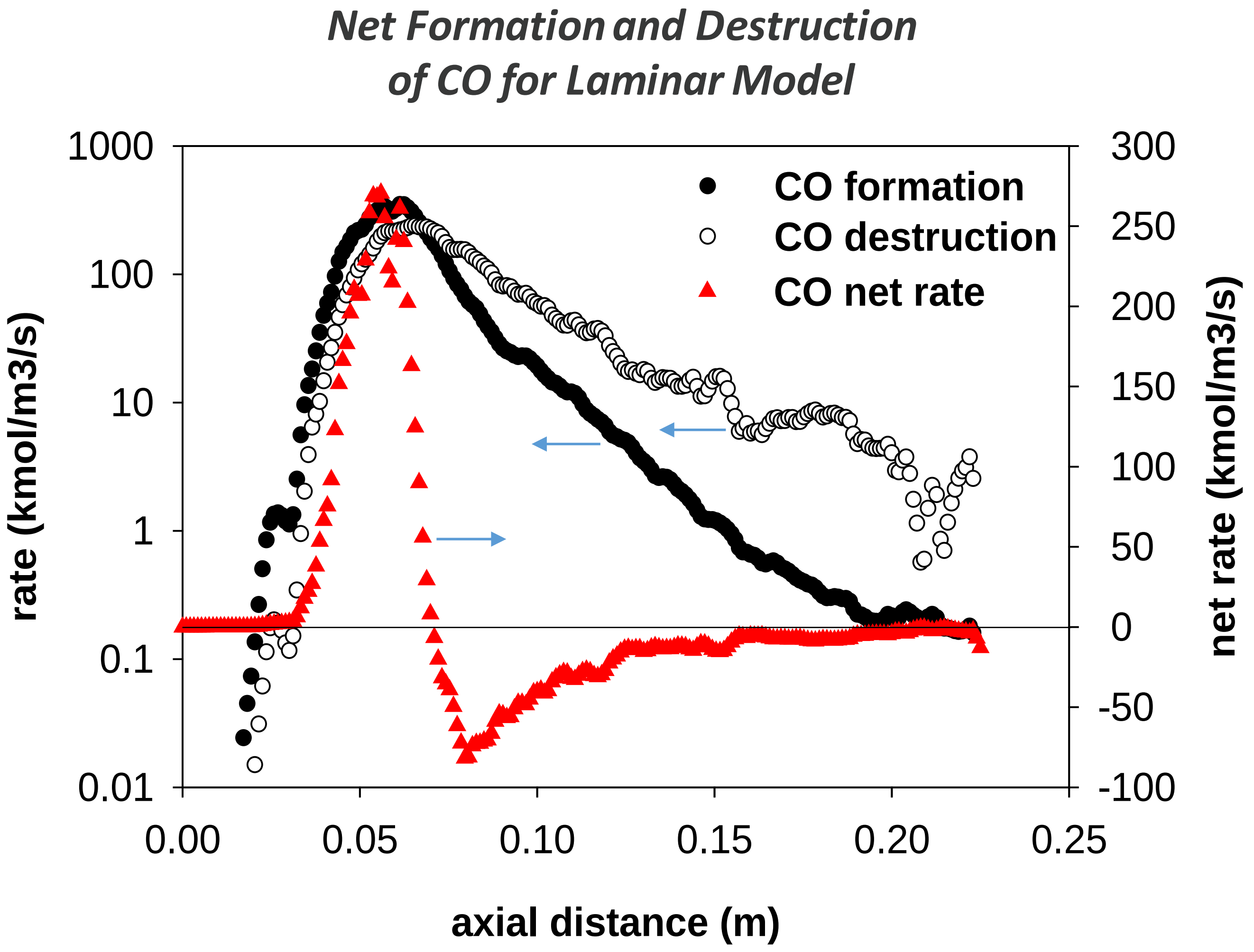


- More rapid decay in CO (and O_2) concentration for FDF model (left plot).
- Right plot shows higher concentrations of unburned fuel for Laminar model (higher CH_4, CH_3, HCO).

Centerline profiles for Case 2 (14% O_2)

Net Formation and Destruction of CO

- CO destruction dominates in post-flame zone but CO formation is still significant.
- “Pockets” of unburned fuel, CH_3 and HCO apparent with laminar model.
- Somewhat counterintuitive since laminar model assumes fast sub-grid mixing.



Mixture Fraction for Case 2 (14% O_2)

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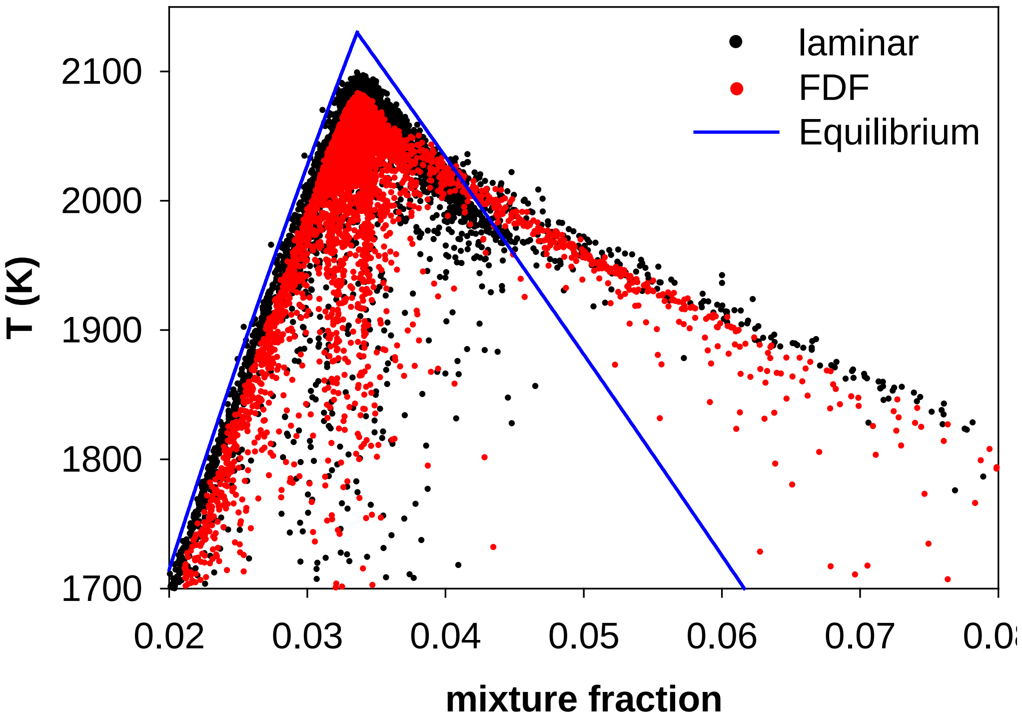
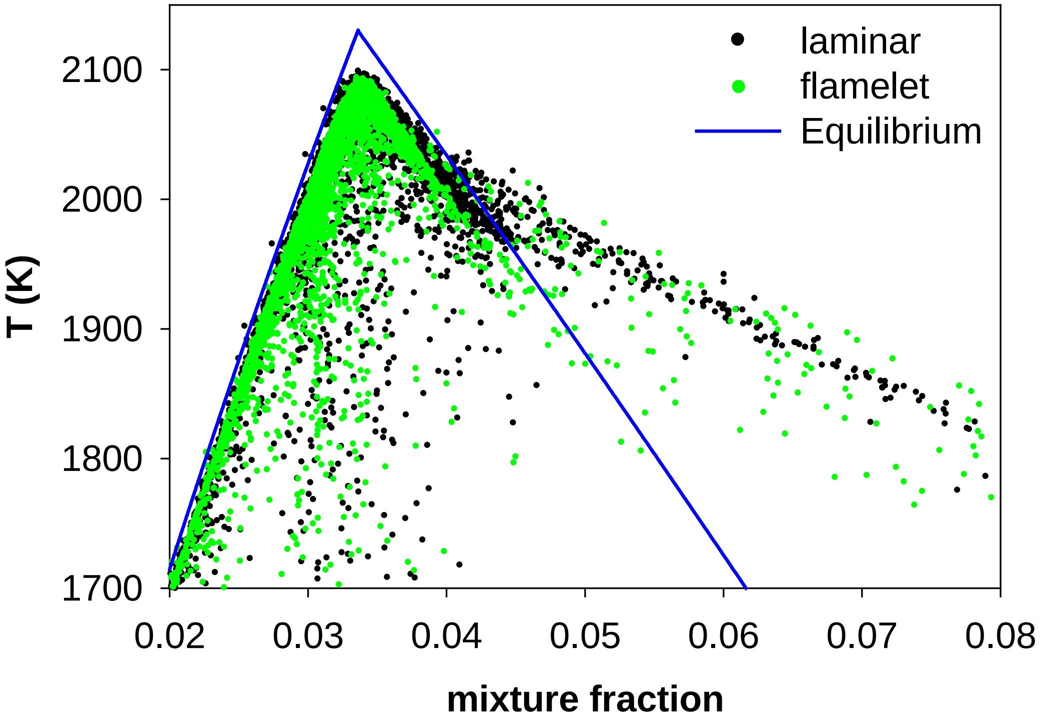
- Instantaneous mixture fraction plots show departure from equilibrium on fuel-rich side.
- Laminar model tends to show higher temperatures (and CO) on fuel-rich side.

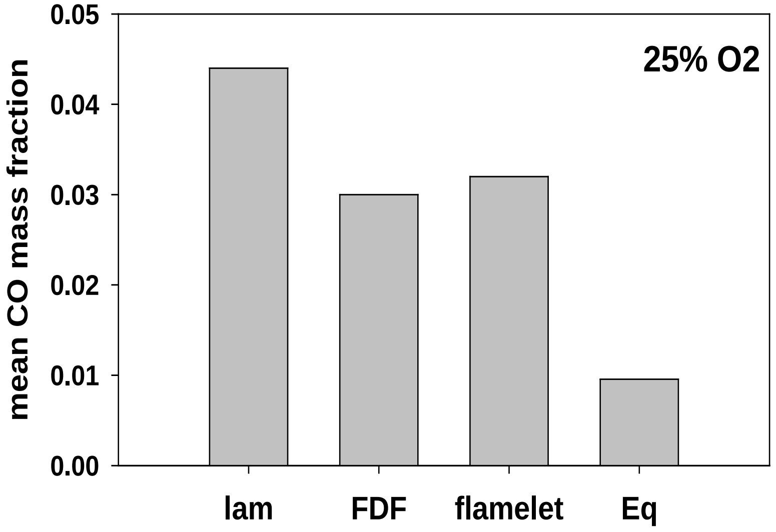


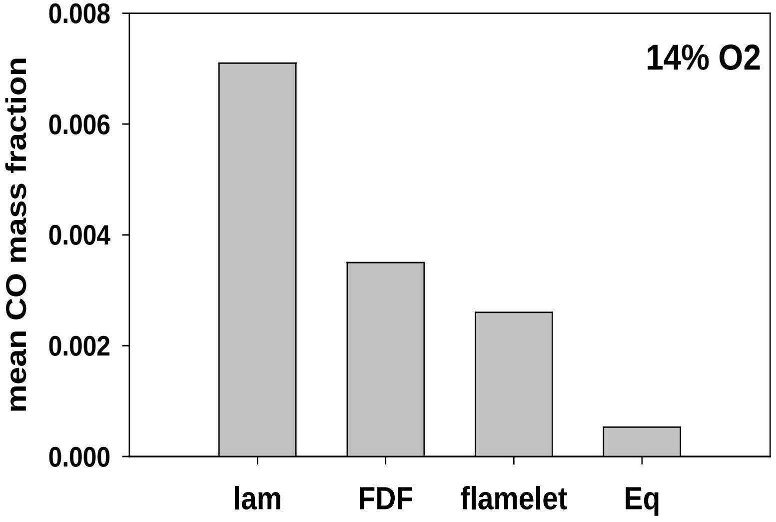


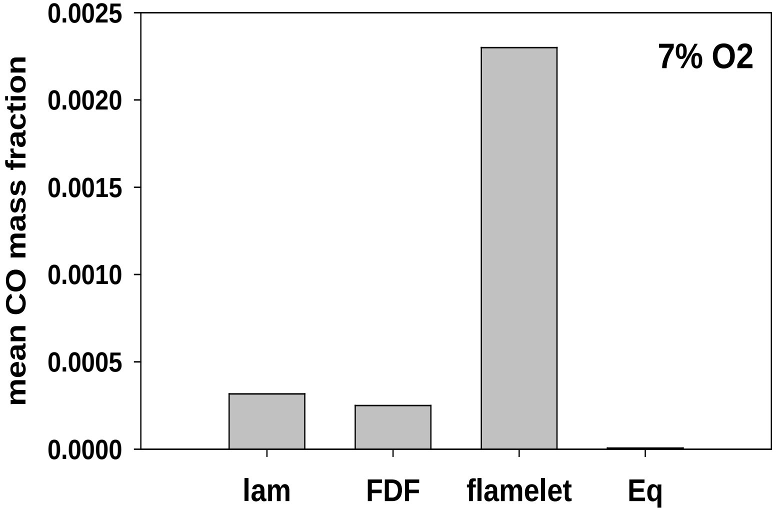
$$Z = \frac{Y_C - Y_{C,O}}{Y_{C,F} - Y_{C,O}}$$

Mean Combustor CO Emissions

- All models predict CO emissions much higher than equilibrium values.
- Laminar model tends to overpredict CO compared to FDF.
- Flamelet model in good agreement with FDF at 25% and 14% O_2 concentration.

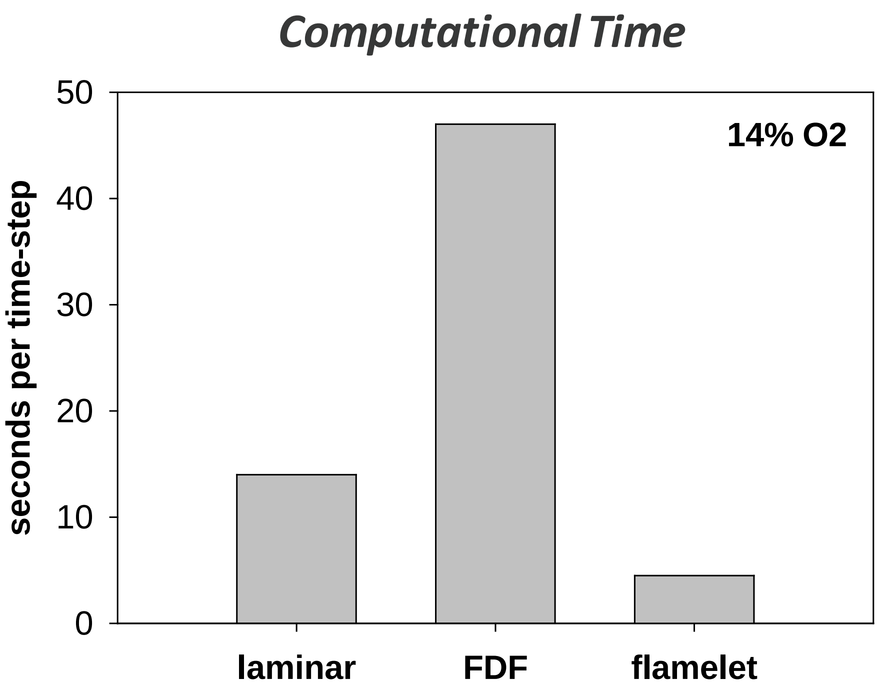






Concluding Remarks

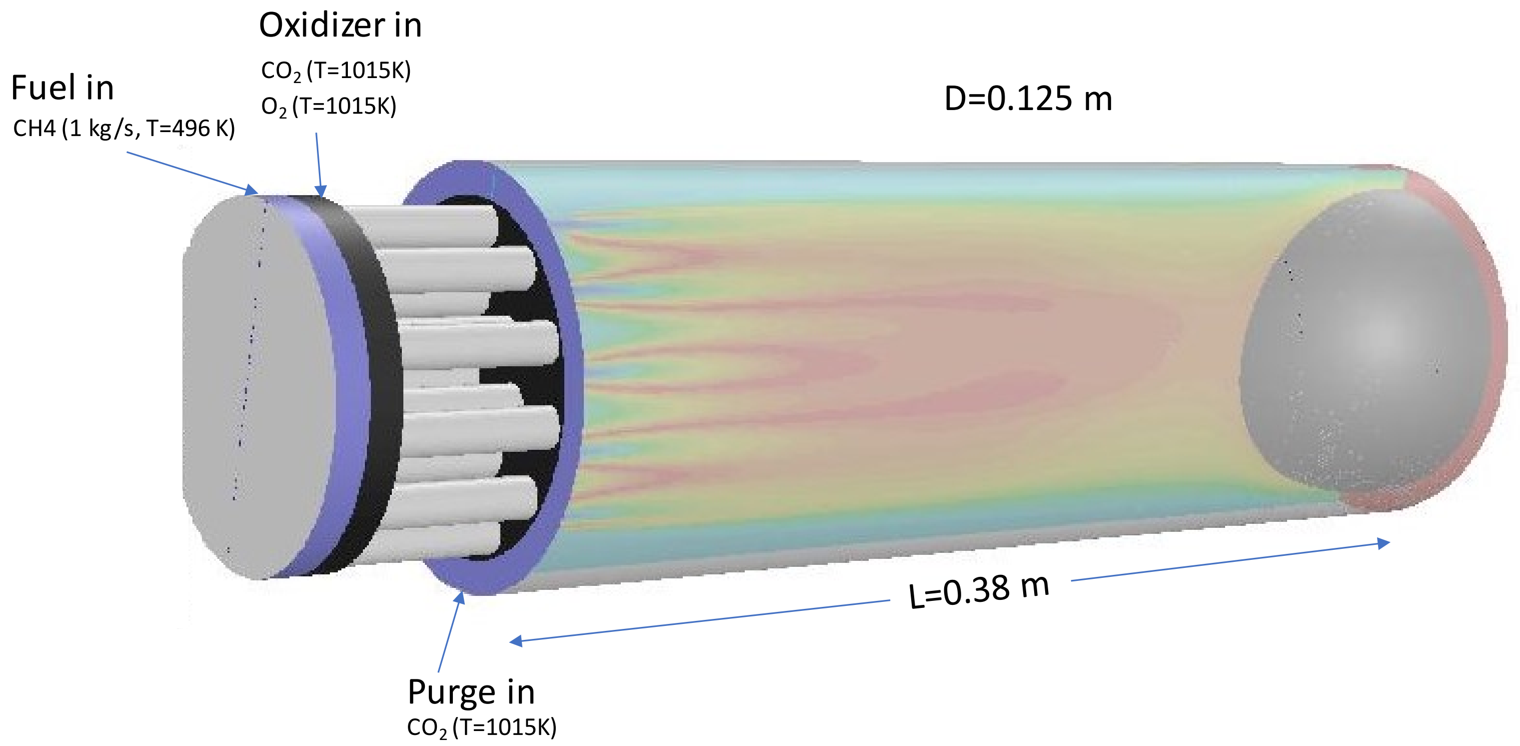
- Decreasing O_2 concentration changes combustion regime from lifted flame to autoignition type of process.
- Combustor CO emissions are a strong function of O_2 concentration (via temperature, OH) and well above equilibrium.
- Flamelet model performed well at 25% and 14% O_2 but can not predict autoignition.
- FDF model provides the most robust treatment of TCI but computationally expensive. Use as a "benchmark case" for comparison.
- Need experimental data for validation!

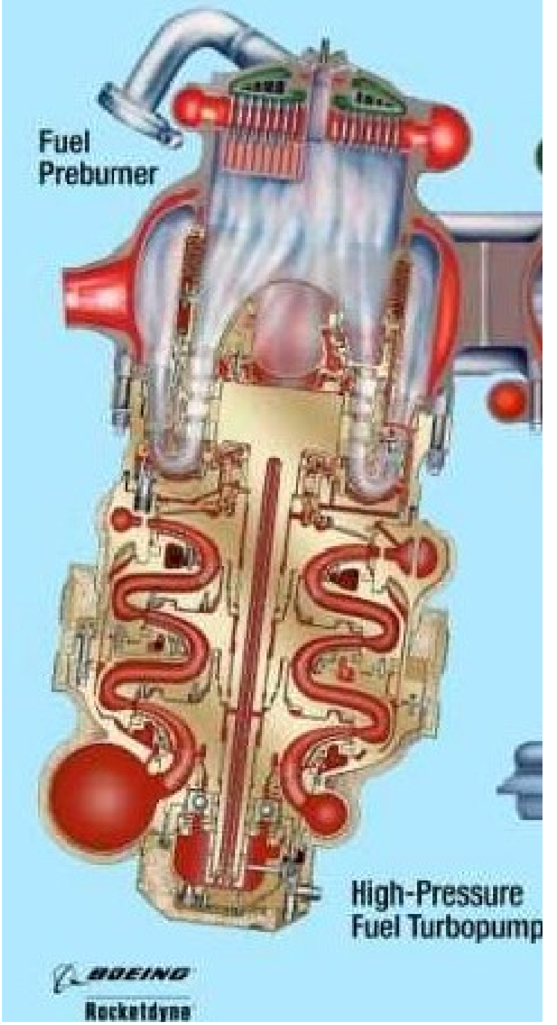


Backup Slides

50 MW Conceptual Combustor

SSME Preburner type combustor – 21 coaxial injectors, 4M Cells

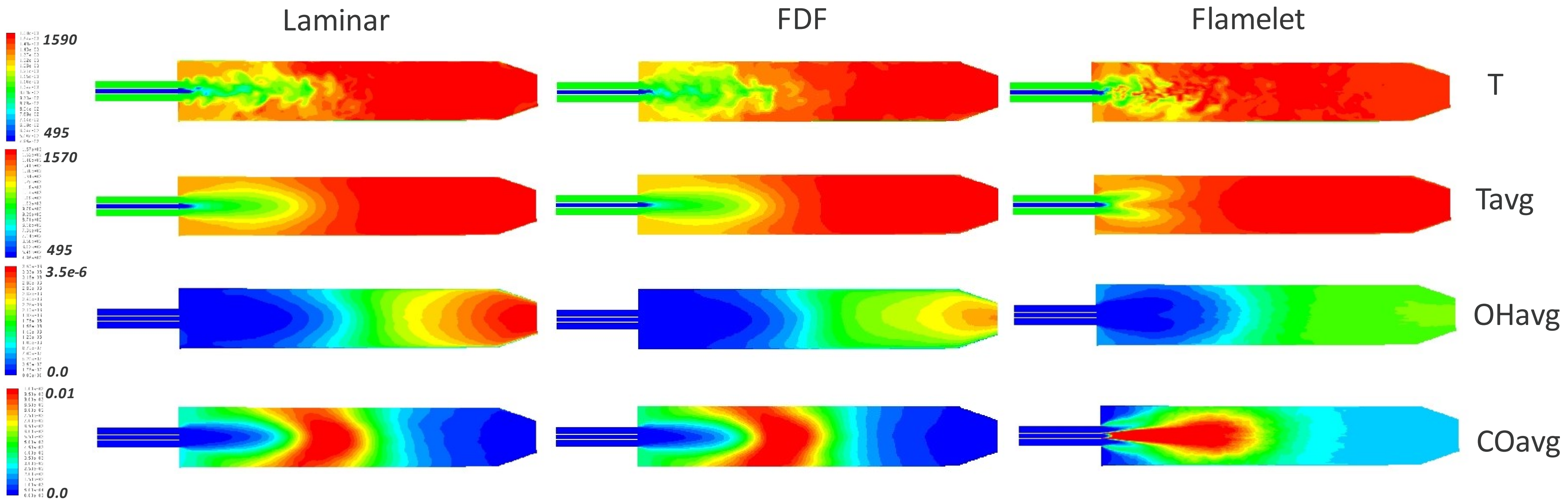




P=300 bar

50 MW Thermal Input

Results for Case 3 (7% O_2)



- FDF and Laminar model show autoignition behavior. Estimated induction time of ~2 msec corresponds to heat release location.
- Flamelet model predicts flame like behavior.