Oxy-Combustion Flame Fundamentals for Supercritical CO2 Power Cycles

Pete Strakey, NETL

NATIONAL ENERGY TECHNOLOGY LABORATORY

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U.S. DEPARTMENT OF ENERGY

Outline

- Effects of pressure and diluents on flames.
- Identification of target conditions.
- Overview of characteristic time and length scales.
- CFD simulations of turbulent time and length scales.
- Chemical kinetic mechanisms.
- LES simulations with varying O_2 concentrations.

Effect of Pressure on Laminar Flame Speed

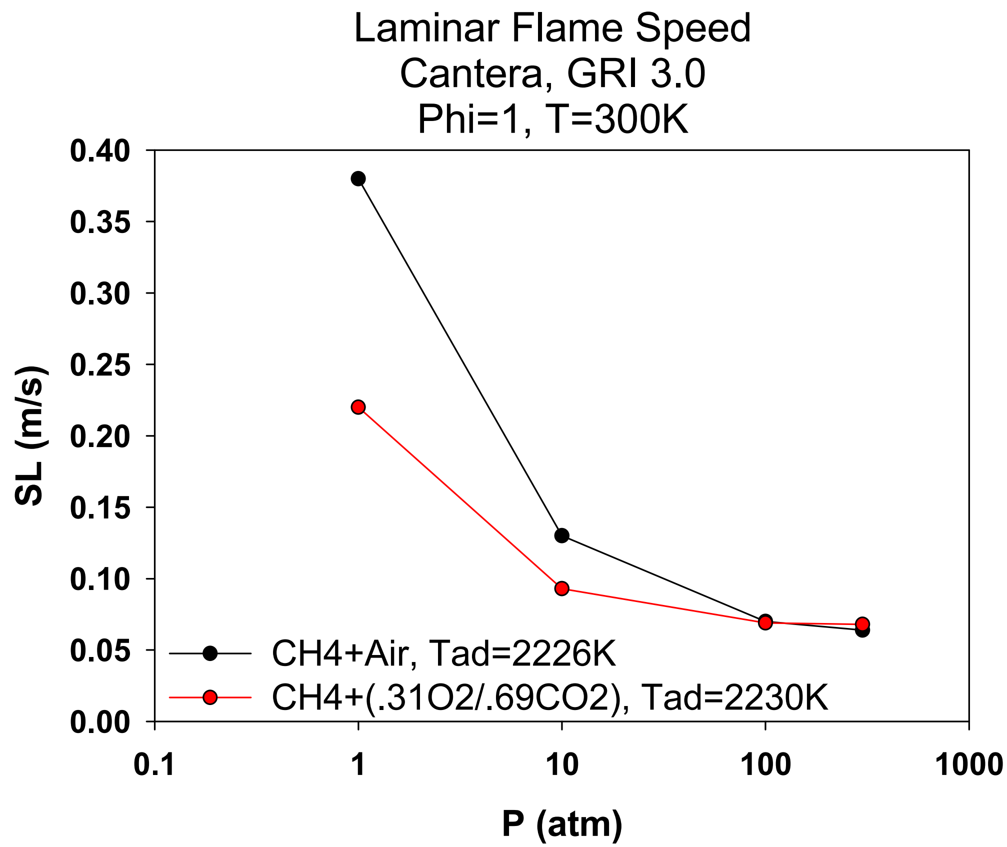
- Cantera with GRI 3.0 used to calculate premixed laminar flame speed.
- Flame speed with 31%O2/69%CO2 lower than air mainly due to lower diffusivity.

$$S_L \propto \sqrt{RR \cdot D}$$

$$D \propto {}^{1}/_{P}$$

RR= Reaction Rate
D= Molecular Diffusivity

- Overall reaction order for CH4/O2/CO2 is ~ 1.4

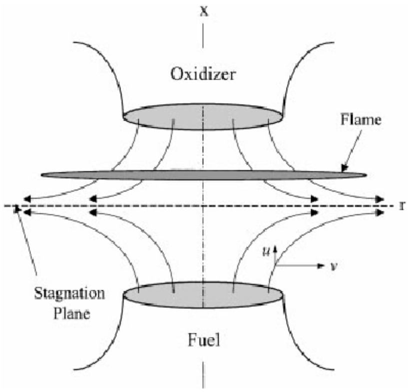


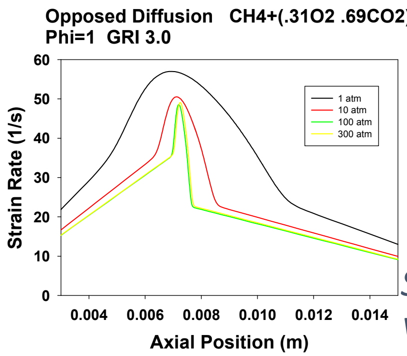
Cantera Non-Premixed Laminar Flame Profiles

- Temperature and OH profiles through flame region.
- Flame thins due to decrease in α being faster than decrease in S_L.
- Peak in OH mole fraction decreases due to three-body recombination reactions.

Laminar Flame Thickness

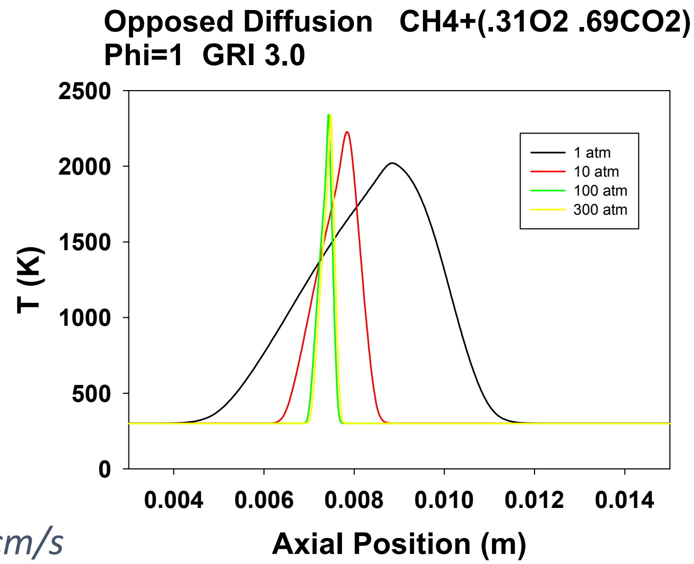
$$\delta_L = \frac{\alpha}{S_L} \qquad \alpha = k/\rho C_P$$

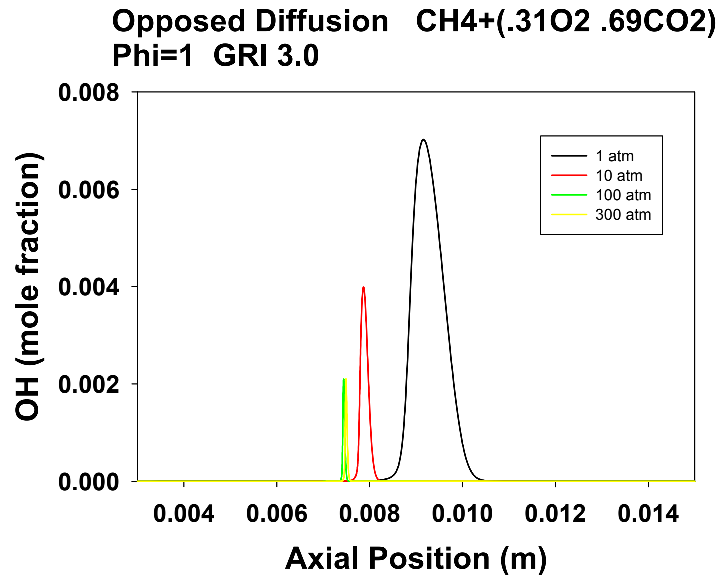




Sep= 2cm

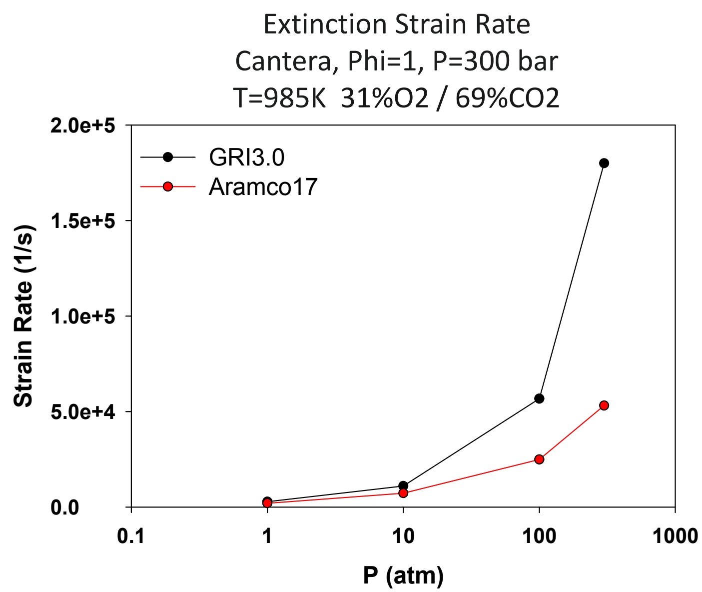
V_F=V_O=27 cm/s

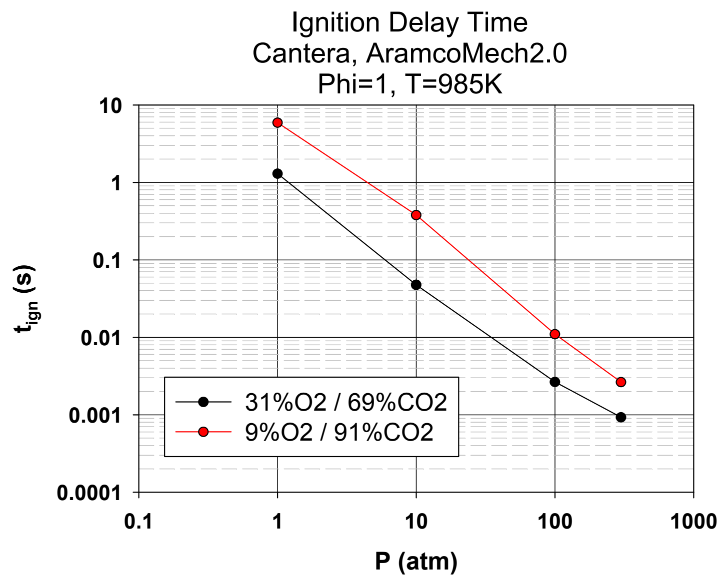




Extinction Strain Rate & Ignition Delay Time

- Extinction strain rate increases with pressure due to flame thinning. Higher strain rate equates to higher turbulence at quenching.
- Significant discrepancy between GRI 3.0 and Aramco. GRI predicts faster kinetics.
- Ignition delay time ranges from 1-3 msec at Allam cycle conditions.





Allam Cycle

- Goal is to estimate some characteristic combustion scales for high pressure oxy-fuel flames for direct-fired sCO2 cycles.
- Target is the Allam cycle conditions (O_2 15% to 30% molar concentration)*.

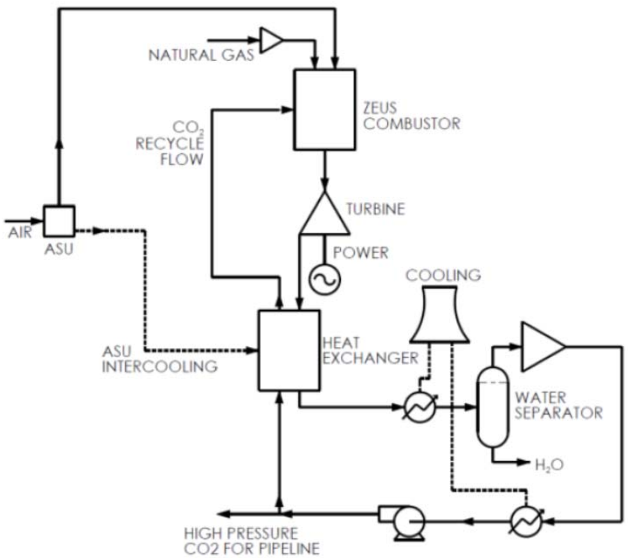


Figure 1. BASIC ALLAM CYCLE NATURAL GAS FLOW DIAGRAM.

Table 1. ALLAM CYCLE KEY POINTS (ISO CONDITIONS)

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

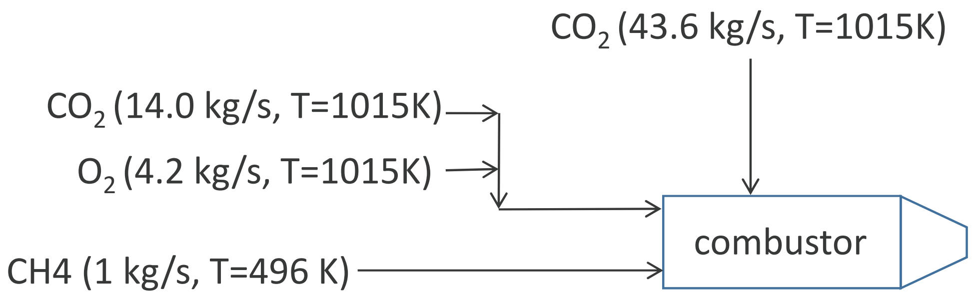
** Allam, et al., Energy Procedia 37, 2013, 1135-1149*

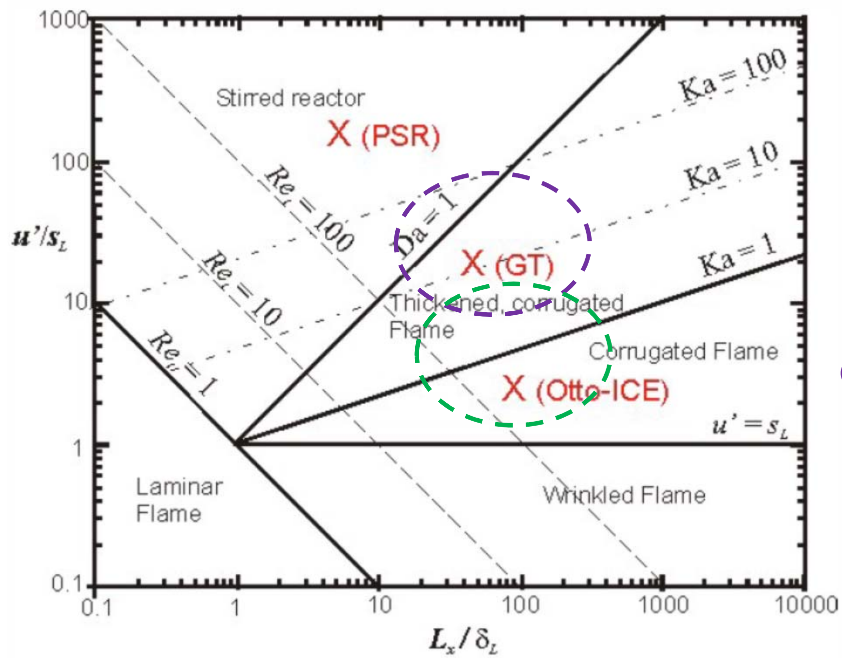
Borghi Combustion Diagram

- Borghi Diagram indicates regime of combustion (wrinkled flames, corrugated flames, stirred reactor, etc.

$$need: \frac{u'}{S_L} \; and \; \frac{l_T}{\delta_L}$$

P=300 bar
50 MW Thermal Input
Phi=0.95





Gas Turbines
IC Engines

Characteristic Scales and Dimensionless Numbers

- **Included here for completeness…**

$$Ka = \frac{\tau_{chem}}{\tau_K} = \frac{\delta_L^2}{l_K^2}$$

Karlovitz Number (chemical time / Kolmogorov time)

K>1 means the smallest eddies can enter and thicken the flame front

$$\mathrm{D}a = \frac{\tau_{turb}}{\tau_{chem}} = .247\left(\frac{k}{\varepsilon}\right)\left(\frac{S_L^2}{\alpha}\right)$$

Damkohler Number (turbulent time / chemical time)

Da>>1 means the chemistry is fast compared to turbulent mixing

$$\delta_L = \frac{\alpha}{S_L}$$

Laminar flame thickness (thermal diffusivity / laminar flame speed)

$$l_K = \left(\frac{v^3}{\varepsilon}\right)^{1/4}$$

Kolmogorov length scale (kinematic viscosity / turbulent dissipation rate)

$$l_T = 0.2\frac{k^{1/2}}{\varepsilon}$$

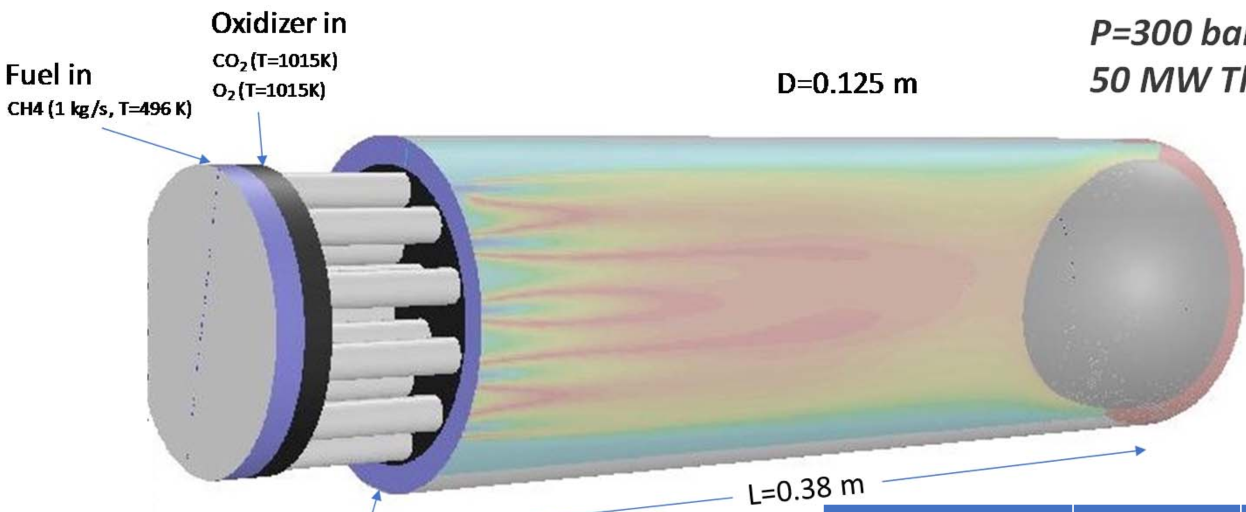
Integral length scale (turbulent kinetic energy / turbulent dissipation rate)

$$u' = \sqrt{\frac{2k}{3}}$$

Turbulent fluctuating velocity

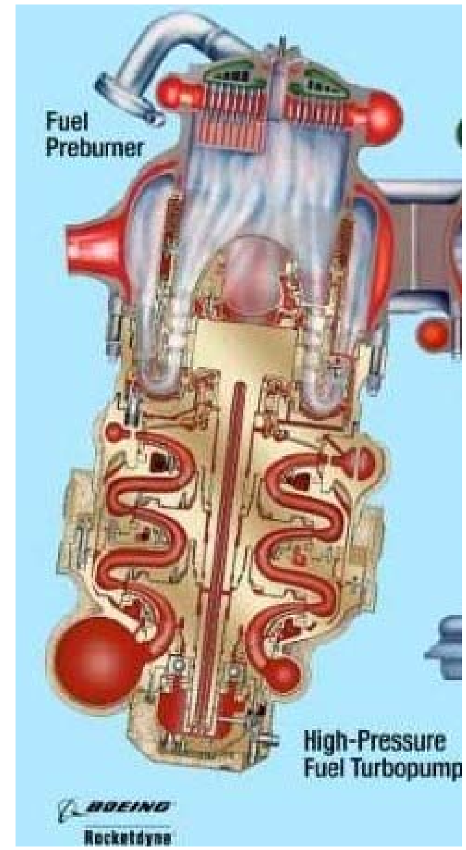
50 MW Conceptual Combustor

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



parameter	Case 1	Case 2	Case 3
O_2 mole fraction	0.31	0.18	0.09
U_{bulk} (m/s)	30	35	70
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)	9.2e-4	1.6e-3	2.5e-3

- ***Flow split of CO_2 between injectors and wall purge was varied to produce cases 1 to 3.***



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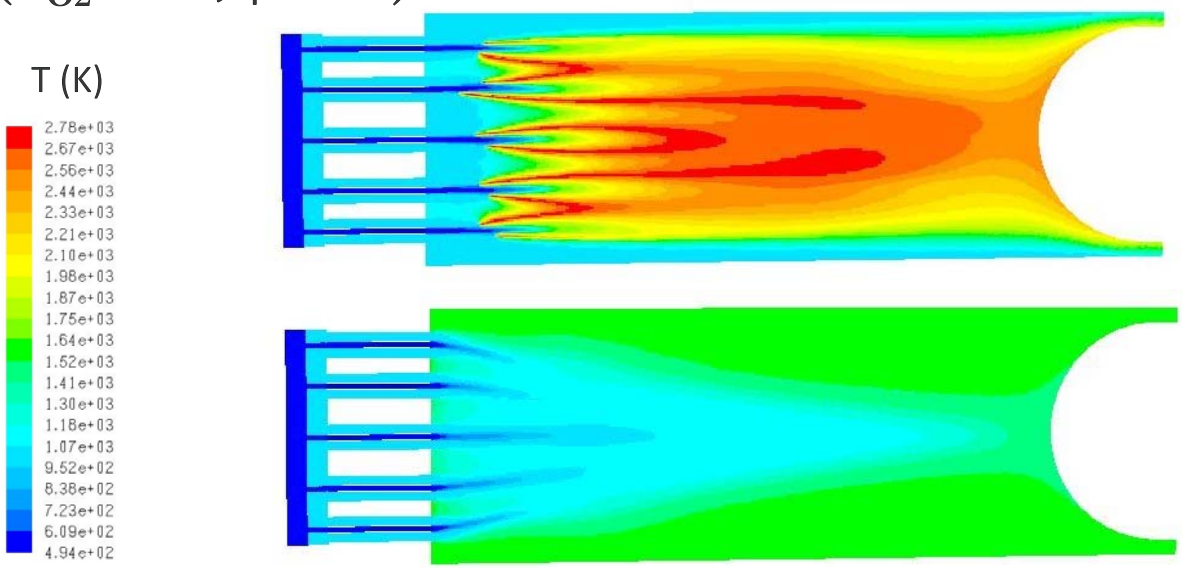
Turbulent Time and Length Scales

Two Limiting Cases:

Case 1: 25% of CO2 by mass mixed in with O2 (X_{O2}=0.31, ϕ=0.95)

Case 3: Fully mixed (100% of CO2 mixed in with O2) (X_{O2}=0.09, ϕ=0.95)

Steady RANS k-e
DRM19 reduced CH4 mechanism
No Combustion model



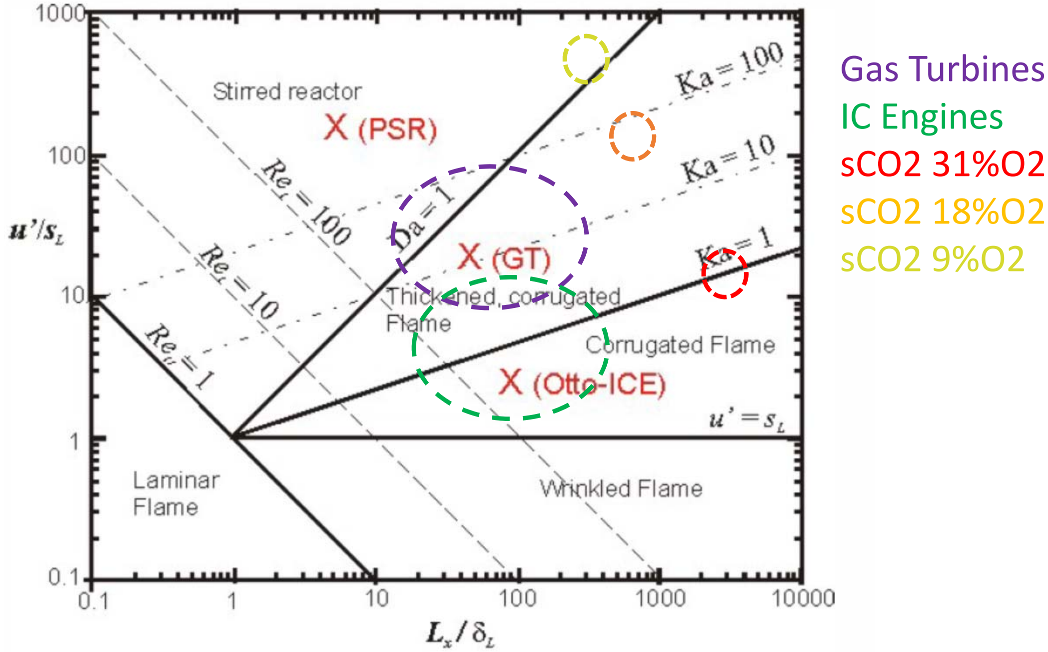
Case 1
25% of CO2 with O2 (X_{O2}=0.31)
75% of CO2 through purge
l_T=1.9 mm
U'=7.5 m/s

Case 3
100% of CO2 with O2 (X_{O2}=0.09)
l_T=2.0 mm
U'=23.8 m/s

Borghi Diagram for Oxy-Combustion

- **Three cases shown for 300 bar oxy-combustion define a range of conditions (O_2 from 9-31%) 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.**



Chemical Kinetic Mechanisms

- No detailed mechanisms validated at sCO2 conditions. Best available is likely Aramco Mech (U. Galway). Validated with flame-speed up to 60 bar and ignition delay to 260 bar. Likely better than GRI 3.0.
- Huge mechanism, 103 species, 480 reactions after reduction to C2 and smaller.
- Need for compact skeletal mechanisms amenable to CFD modeling (10-30 species maximum).

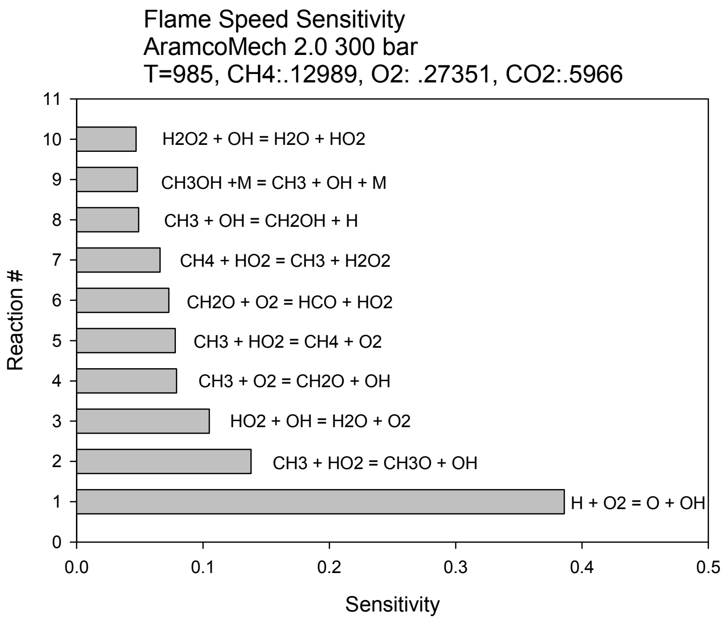
Need flame speed, species profiles and induction time data for direct-fired conditions!

Mechanism Reduction

- Combination of reaction path analysis, flame-speed sensitivity and ignition delay time sensitivity.
- Optimized for Allam cycle combustor conditions
  - 300 bar
  - $T_{preheat}$ ~ 1000K
  - Oxidizer: 25% O_2 + 75% CO_2

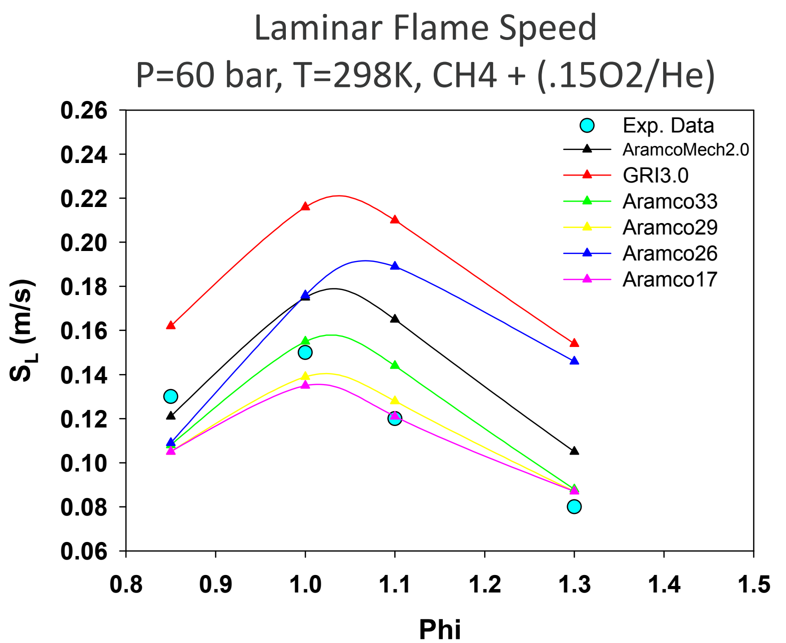
- Several skeletal mechanisms developed with 33, 29, 26 and 17 species.

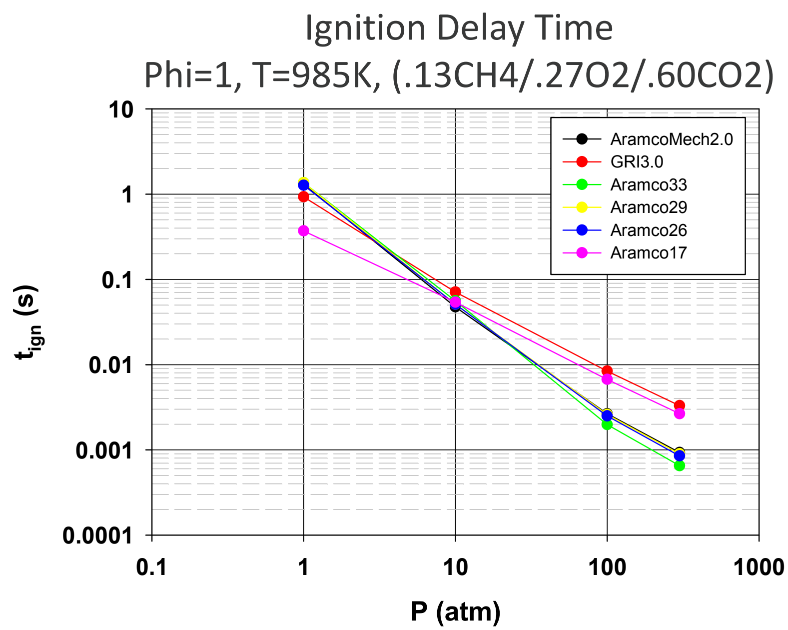
Flame speed sensitivity at 300 bar



Mechanism Reduction

- **Performance comparison of various skeletal mechanisms.**
  - Flame speed and ignition delay improve with the inclusion of more species and reactions.
    - 33 species mechanism able to predict flame-speed and ignition delay fairly well.
    - 17 species able to predict flame-speed to within ~30% of detailed mechanism.

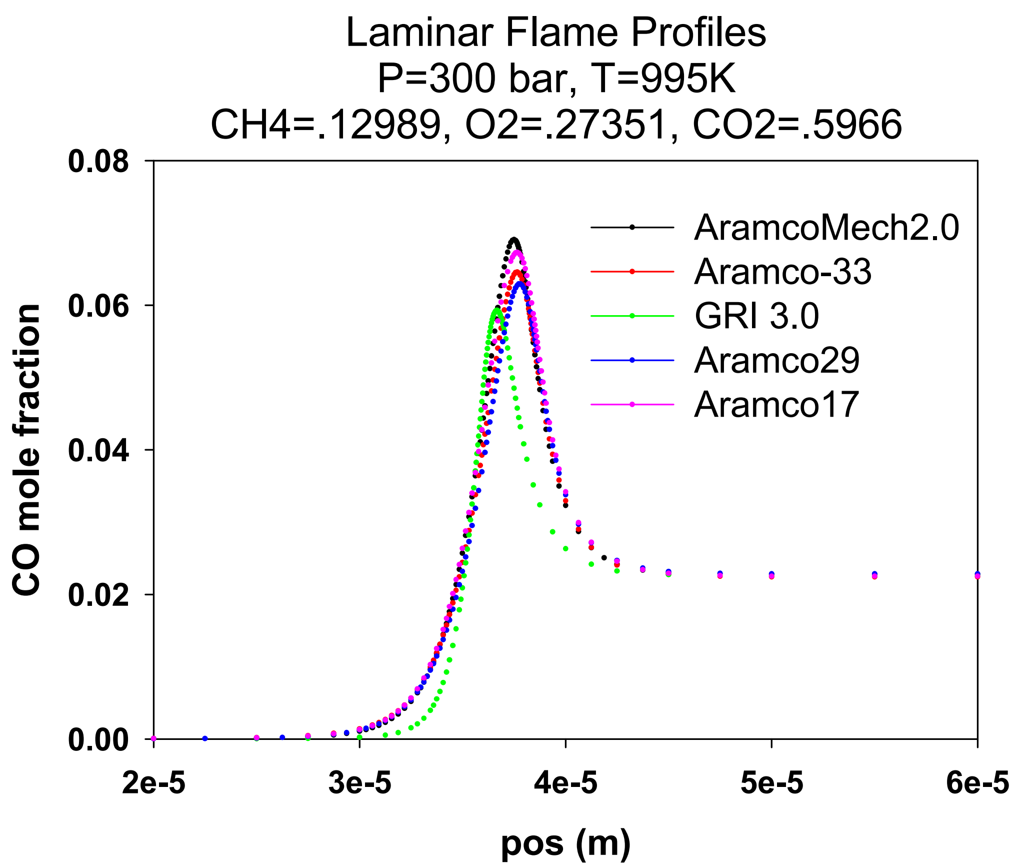




Rozenchan, et al. Proc. Comb. Inst., Vol. 29, 2002, pp. 1461-1469.

Mechanism Reduction

- **Performance comparison of various skeletal mechanisms.**
  - All do very well for CO production profiles.
- **CO prediction important for accurate cycle efficiency calculations.**

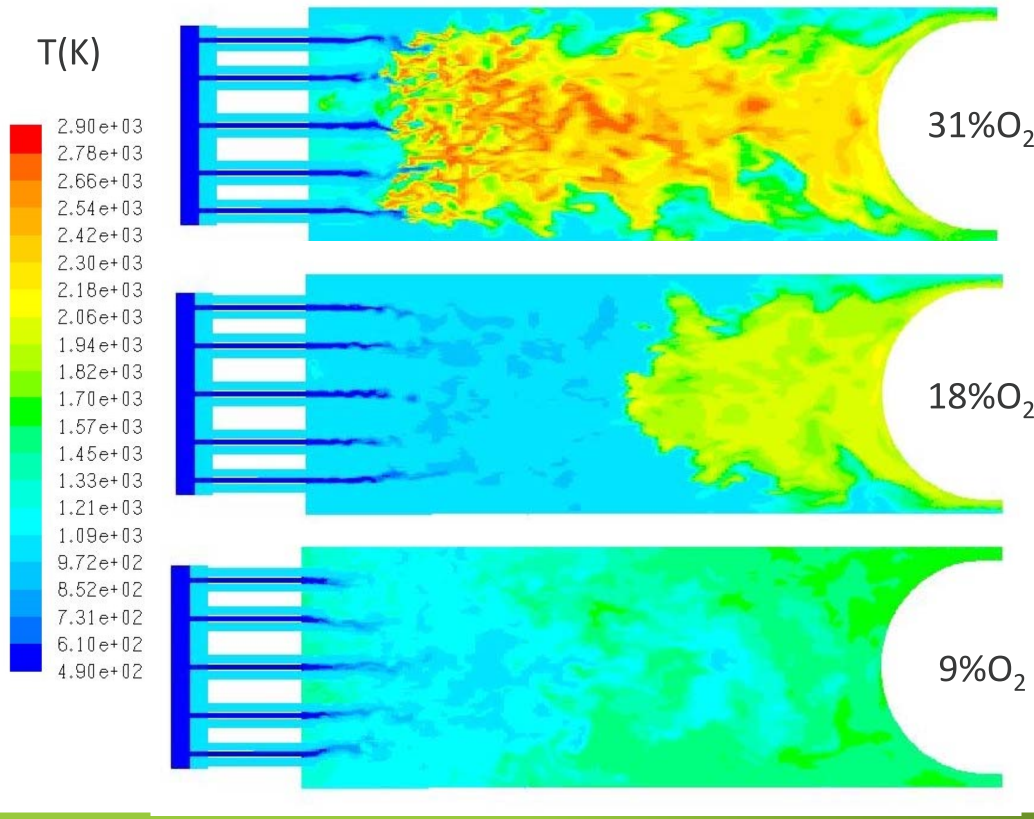


LES Modeling: Temperature Contours

Large Eddy Simulation, Dynamic k-e transport
17-species skeletal mechanism
No Combustion Model
Phi=0.95

- **Combustor exit temperature is the same for all three cases (~1520 K).**
- **Combustion transitions from lifted flame to stirred reactor as O_2 is decreased. Consistent with Borghi diagram.**
  - Peak temperature decreases (2730 K to 1614 K).
  - Core velocity increases (30 m/s to 70 m/s).

Temperature Snapshots at Quasi-Steady Conditions

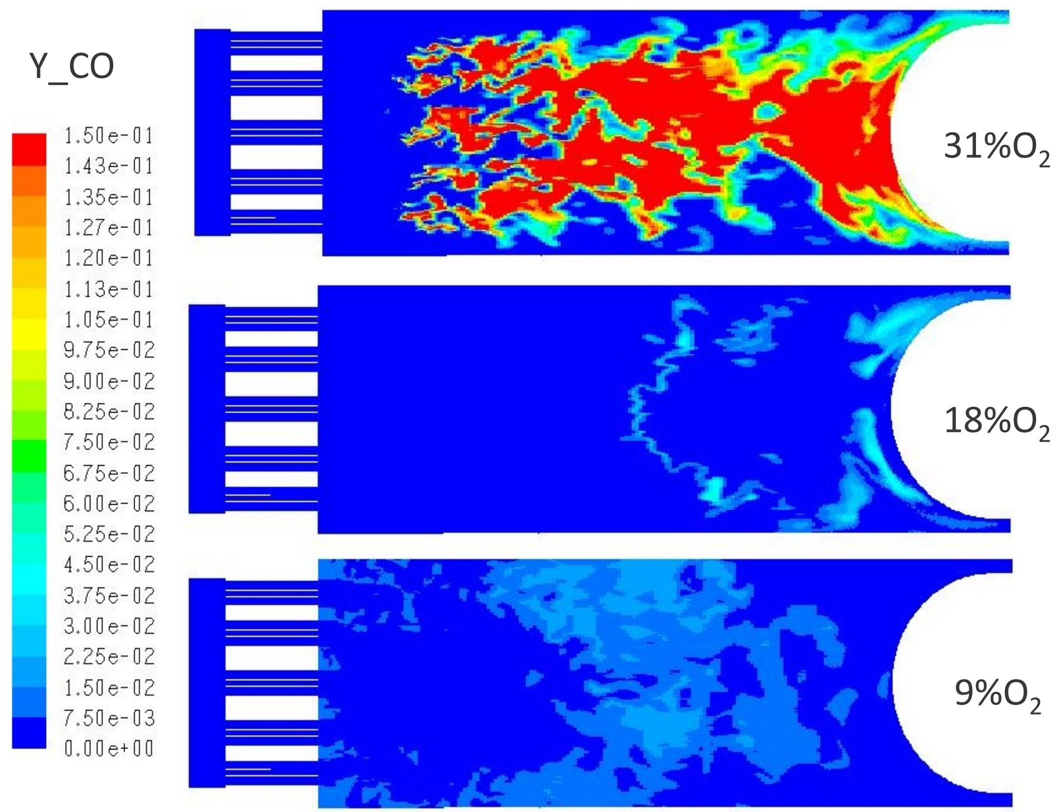


LES Modeling: CO Contours

Large Eddy Simulation, Dynamic k-e transport
17-species skeletal mechanism
No Combustion Model
Phi=0.95

- Combustor exit temperature is the same for all three cases (1520 K).
- For 31% O_2 case, peak CO concentration well above equilibrium value (X_{CO}=0.25).
- For all cases, peak CO is significantly higher than equilibrium.

CO Mass Fraction Snapshots at Quasi-Steady Conditions



LES Modeling: CO Summary

Case	Oxidizer flow (kg/s)	Purge flow (kg/s)	O2 mole %	Equilibrium Flame Temp(K)	Equilibrium Flame CO mole %	LES Peak Temp(K)	LES Peak CO Mole %	LES Avg CO mole %
1	16.8	43.6	31.0	2690	2.4	2730	25.0	3.5
2	30.4	30.0	18.0	2100	0.15	2060	5.0	1.0
3	60.4	0.0	9.0	1612	0.0018	1614	3.0	0.013

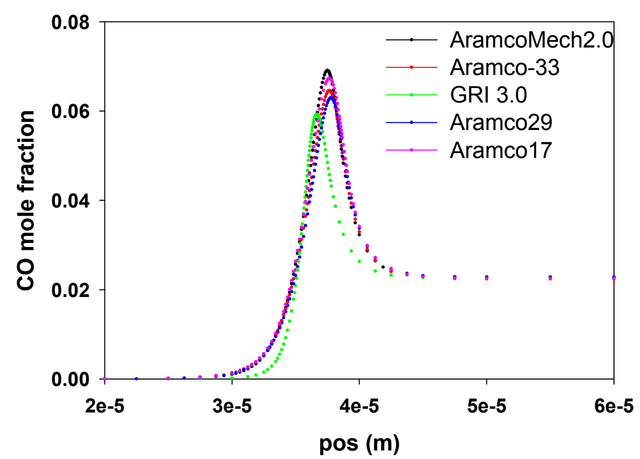
Equilibrium Calcs

Comb Exit:

T=1612 K

X_{CO} = 0.0018 %

- Peak CO concentrations well above equilibrium levels.
- Average CO concentrations at combustor exit also well above equilibrium levels.
- Cycle efficiency calculations indicate roughly a 0.75 % pt. drop in efficiency per mole % CO in working fluid.



Concluding Remarks

- **Oxy-combustion at 300 bar is somewhat uncharted territory.**
  - Conditions more representative of rocket engines.
  - Limited data available.
- **Need for validated detailed chemical kinetic mechanisms as well as reduced mechanisms.**
- **Must take care in selecting appropriate combustion models (fast mixing, flamelet, EDC, PDF, etc…).**
- **CO production highly sensitive to flame temperature and may be well above equilibrium.**